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STATISTICS OF 1-DIMENSIONAL ATOM MOTION WITH NEXT-NEAREST NEIGH--ETC(U)

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STATISTICS OF 1-DIMENSIONAL ATOM MOTION WITH NEXT NEAREST NEIGHBOR TRANSITIONS

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During the last decade considerable progress has been made in understanding the self-diffusion of metal atoms on well defined crystal planes. This advance has occurred through the use of the field ion microscope, which makes it possible to visualize individual atoms, and to prepare highly perfect surfaces. With this microscope it is possible to determine by direct observation the mean square displacement of atoms adsorbed at a surface, and thus to derive their diffusion coefficient D from Einstein's relation.

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STATISTICS OF 1-DIMENSIONAL ATOM MOTION WITH NEXT-NEAREST NEIGHBOR TRANSITIONS*

by

Mark Erickson Twigg†

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†Supported in part by the Joint Services Electronics Program (U.S. Army, U.S. Navy and U.S. Air Force) under Contract DAAB-07-72-C-0259.

STATISTICS OF 1-DIMENSIONAL ATOM MOTION WITH NEXT-NEAREST NEIGHBOR TRANSITIONS

BY

MARK ERICKSON TWIGG

B.S., University of Maryland, 1974

THESIS

Submitted in partial fulfillment of the requirements
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INTRODUCTION

During the last decade considerable progress has been made in understanding the self-diffusion of metal atoms on well defined crystal planes [1]. This advance has occurred through the use of the field ion microscope, which makes it possible to visualize individual atoms, and to prepare highly perfect surfaces. With this microscope it is possible to determine by direct observation the mean square displacement of atoms adsorbed at a surface, and thus to derive their diffusion coefficient D from Einstein's relation, which for one-dimensional motion assumes the form [2]

$$\langle(\Delta R)^2\rangle = 2Dt \quad . \tag{1}$$

A considerable fund of information about the directionality of surface diffusion, about the role of surface structure, and about the energetics of atomic jumps has been built up this way. Despite that, very little is known about the actual atomic motions involved in the diffusion process.

It is by now customary to assume that in moving over a surface an atom hops, at random moments in time, from one site to an adjacent nearest neighbor site. For the sake of simplicity we shall confine ourselves to one-dimensional motion only, and postulate that the surface sites are separated from each other by a distance ℓ. The probability that an atom will be at a distance $n\ell$ from the origin after a time t is then given, in terms of the rate α at which jumps occur in one direction, by [3]

$$p_n(t) = \exp(-2\alpha t)I_n(2\alpha t) \quad , \tag{2}$$

where $I_n(x)$ is the modified Bessel function of order n. The mean square displacement $\langle(\Delta R)^2\rangle$ is then

$$\langle(\Delta R)^2\rangle = 2\alpha t\ell^2 \ . \tag{3}$$

The validity of this model cannot be established from an examination of the mean square displacement alone. This requires a detailed comparison of the probability density, determined from experiments, with the values predicted by Eq. (2). One such comparison has been made [4], for the behavior of Re atoms on the (211) plane of tungsten. Within the sizable statistical error, arising from the limited data set, it appears that Eq. (2) is adequate to describe the actual diffusion process.

It still remains to be established, however, that surface diffusion involves only jumps between nearest neighbors. With the data available right now, it is not possible to exclude the possibility that occasionally, an atom might carry out a jump spanning two nearest neighbor spacings instead of just one. The aim of this thesis is to examine the feasibility of detecting such double jumps in diffusion measurements. To this end we idealize the one-dimensional diffusion of an adatom as involving single as well as double jumps at random moments, the former occurring at a rate 2α, the latter at a rate 2β. The statistical consequences of this model are developed in Chapter I; Chapter II, is devoted to a detailed discussion of the conditions that must be satisfied in an experiment designed to measure the contributions of multiple jumps. Especially important in these considerations are estimates of the statistical errors involved in such determinations. These estimates rely on a fairly complicated mathematical apparatus; this is developed, at some length, in separate appendices.

I. RELATION BETWEEN PROBABILITY DENSITIES, JUMP RATES, AND MOMENTS

Oddly enough, the behavior of random walks involving jumps of different lengths has been neglected in the literature. Lakatos-Lindenberg and Schuler [5] have examined the statistics of a particle making transitions to both nearest and next-nearest neighbor sites; however, they considered only jumps at fixed time intervals, a model which is not strictly appropriate to actual diffusion processes. We will therefore develop here the consequences of extending the usual model for one-dimensional diffusion, in which atoms are presumed to execute jumps after random time intervals, by allowing displacements both between nearest and next-nearest neighbors. Transitions in a given direction are presumed to occur at a rate α to the nearest neighbor site, and at a rate β to the next-nearest neighbor. Motion to the right and to the left is equally probable.

A. Probability Densities and Jump Rates

The first step in developing our model is to find the probability that an adatom starting at a site m be at site n after a time t. We designate this probability as $p_n^m(t)$ and find it via the Kolmogorov equation, which for this system assumes the form [6]

$$\frac{dp_n^m}{dt} = \beta p_{n-2}^m + \alpha p_{n-1}^m - 2(\alpha+\beta)p_n^m + \alpha p_{n+1}^m + \beta p_{n+2}^m \quad ; \qquad (4)$$

here α is the rate at which adatoms execute unit displacements and β is the rate at which adatoms execute double displacements. The distance ℓ between adjacent sites is taken to be unity.

In order to solve the Kolmogorov equation and thereby find the probability density $p_n^m(t)$, we need to uncouple the time variable from the position variables. This is accomplished by the use of the well known generating function for the probability density. The generating function $G(t,z)$ is defined as

$$G(t,z) = \sum_n z^n p_n^m(t) \ . \tag{5}$$

The symbol $\sum_n$ is throughout used to designate summation over the limits $n = -\infty$ to ∞, that is

$$\sum_n \equiv \sum_{n=-\infty}^{\infty} \ .$$

We use Eqs. (4) and (5) to derive a simple differential equation involving $G(t,z)$. Once the generating function has been obtained from this, $p_n^m(t)$ can be found using the definition in Eq. (5).

To derive the differential equation for $G(t,z)$, we note that z is time independent; it therefore follows from Eq. (5) that

$$\frac{\partial G}{\partial t}(t,z) = \sum_n z^n \frac{dp_n^m(t)}{dt} \ . \tag{6}$$

Multiplying the Kolmogorov equation by z^n and summing over n, we find that

$$\frac{\partial G(t,z)}{\partial t} = \sum_n z^n \{\beta p_{n-2}^m + \alpha p_{n-1}^m - 2(\alpha+\beta) p_n^m + \alpha p_{n+1}^m + \beta p_{n+2}^m\} \ . \tag{7}$$

Note that

$$\sum_n z^n p_{n-2}^m = z^2 \sum_n z^n p_n^m \tag{8a}$$

$$\sum_n z^n p_{n-1}^m = z \sum_n z^n p_n^m \tag{8b}$$

$$\sum_n z^n p^m_{n+1} = z^{-1} \sum_n z^n p^m_n \tag{8c}$$

$$\sum_n z^n p^m_{n+2} = z^{-2} \sum_n z^n p^m_n \ . \tag{8d}$$

From these five equations above, we conclude that

$$\frac{\partial G(t,z)}{\partial t} = \sum_n z^n \{\beta z^2 p^m_n + \alpha z p^m_n - 2(\alpha+\beta) p^m_n + \frac{\alpha}{z} p^m_n + \frac{\beta}{z^2} p^m_n \} \ . \tag{9}$$

This can be written more simply as

$$\frac{\partial G(t,z)}{\partial t} = \sum_n z^n p^m_n \{\beta(z^2 + z^{-2}) + \alpha(z + z^{-1}) - 2(\alpha+\beta)\} \ . \tag{10}$$

Recalling the definition of $G(t,z)$ in Eq. (5), Eq. (10) can also be written as

$$\frac{\partial G(t,z)}{\partial t} = G(t,z)\{\beta(z^2 + z^{-2}) + \alpha(z + z^{-1}) - 2(\alpha+\beta)\} \ . \tag{11}$$

It is apparent that the differential equation for the generating function is much simpler than the original Kolmogorov relation. Equation (11) has the simple solution,

$$G(t,z) = C \exp\{[\beta(z^2 + z^{-2}) + \alpha(z + z^{-1}) - 2(\alpha+\beta)]t\} \ .$$

The constant C can be found from the boundary conditions. Given that the adatom begins its random journey at m, we know that

$$p^m_n(t=0) = \delta_{nm} \ ,$$

where δ_{nm} is Kronecker's delta. Therefore

$$G(t=0,z) = \sum_n \delta_{nm} z^n = z^m$$

and

$$G(t,z) = z^m \exp\{[\beta(z^2 + z^{-2}) + \alpha(z + z^{-1}) - 2(\alpha+\beta)]t\} \ . \tag{12}$$

In order to determine the probability density $p_n^m(t)$, we must expand $G(t,z)$ in a Laurent series. This can be done using the Schlömilch series [7].

$$\exp\left[\frac{x}{2}(y+y^{-1})\right] = \sum_n y^n I_n(x) \ . \qquad (13)$$

This allows us to express $G(t,z)$ as a series involving modified Bessel functions I_n of order n. Equation (12) can be written in the equivalent form

$$G(t,z) = z^m \exp\{\beta t[z^2+z^{-2}]\} \exp\{\alpha t[z+z^{-1}]\} \exp\{-2(\alpha+\beta)t\} \ . \qquad (14)$$

According to Eq. (13); however,

$$\exp\{\beta t[z^2+z^{-2}]\} = \sum_{n_1} I_{n_1}(2\beta t) z^{2n_1},$$

$$\exp\{\alpha t[z+z^{-1}]\} = \sum_{n_2} I_{n_2}(2\alpha t) z^{n_2} \ .$$

From the definition of the generating function, in Eq. (5), it follows that

$$G(t,z) = \sum_n p_n^m z^n$$

$$= \exp[-2(\alpha+\beta)t] \sum_{n_1 n_2} I_{n_1}(2\beta t) I_{n_2}(2\alpha t) z^{(2n_1+n_2+m)} \ . \qquad (15)$$

Identifying n as

$$n = 2n_1 + n_2 + m \ ,$$

we have

$$n_2 = (n-m) - 2n_1 .$$

From Eq. (15) the probability density $p_n^m(t)$ can now be written as

$$p_n^m(t) = e^{-2(\alpha+\beta)t} \sum_k I_k(2\beta t) I_{(n-m)-2k}(2\alpha t) \ , \qquad (16)$$

where k has been substituted for n_1, the dummy variable. When only unit displacements occur, $\beta = 0$ and

$$p_n^m(t) = e^{-2\alpha t} \sum_k I_k(0)\, I_{(n-m)-2k}(2\alpha t) \; .$$

Note that $I_k(0) \neq 0$ if and only if $k = 0$; for that case $I_o(0) = 1$, so that

$$p_n^m(t) = e^{-2\alpha t}\, I_{(n-m)}(2\alpha t) \tag{17}$$

for $\beta = 0$. This agrees with the standard expression for an adatom diffusing via unit displacements. When only double displacements are allowed,

$$\begin{aligned} p_n^m(t) &= e^{-2\beta t} \sum_k I_k(2\beta t)\, I_{(n-m)-2k}(0) \\ &= e^{-2\beta t} I_{(n-m)/2}(2\beta t) \end{aligned} \tag{18}$$

for $\alpha = 0$; here n-m must be an even integer.

B. Jump Rates and Moments

In order to determine the rates β and α at which a diffusing adatom makes double and single displacements, we must reduce the above equations into explicit expressions for observable quantities. Such quantities are the moments μ_r' of the displacements executed by the adatom in the one dimensional walk.

Suppose that an adatom is initially at position m_1. We allow t seconds for the adatom to perform a random walk and call its position at the end of the walk n_1. The i-th initial and final positions that we observe will be designated by m_i and n_i. On M occations m_i and n_i are recorded; we are thus able to define M displacements x_i, where

$$x_i = (m_i - n_i) \; . \tag{19}$$

If we were to make an arbitrarily large number of observations we would be able to find μ'_r, the r-th moment about zero, which is defined as

$$\mu'_r = \lim_{M\to\infty} \frac{1}{M} \sum_{i=1}^{M} (x_i)^r \ . \tag{20a}$$

As shown in Appendix B, the r-th moment about the mean

$$\mu_r = \lim_{M\to\infty} \frac{1}{M} \sum_{i=1}^{M} (x_i - \mu'_1)^r \tag{20b}$$

is often a more useful quantity than μ'_r. The one dimensional random walk is symmetric about the adatom's initial position, so the odd moments about zero vanish in the limit of an infinite number of observations. Because the mean μ'_1 is an odd moment and therefore zero, we know from Eqs. (20a) and (20b) that for our example

$$\mu_r = \mu'_r \ . \tag{21}$$

In order to find these moments in terms of the jump rates α and β, we must seek a way of relating the moments to the generating functions given by Eqs. (5) and (12), that is to

$$\begin{aligned} G(t,z) &= \sum_n p_n^m(t) z^n \\ &= z^m \exp\{[\beta(z^2 + z^{-2}) + \alpha(z + z^{-1}) - 2(\alpha + \beta)]t\} \ . \end{aligned}$$

From Eq. (20a) we know that the mean displacement for the adatom performing the random walk is

$$\mu'_1 = \lim_{M\to\infty} \frac{1}{M} \sum_{i=1}^{M} x_i \ . \tag{22}$$

We also know that the probability for the diffusing adatom to occupy site n, having started at site m t seconds earlier, is $p_n^m(t)$. An equivalent expression for the mean position of the adatom is then

$$\mu_1' = \sum_n n\, p_n^m(t) \quad . \tag{23}$$

The similarity between the relation for the generating function and for the mean causes us to realize that

$$\frac{\partial}{\partial z} G(t,z) = \sum_n p_n^m(t) n z^{n-1}$$

$$(z \frac{\partial}{\partial z})\ G(t,z) = \sum_n n\, p_n^m\, z^n$$

$$(z \frac{\partial}{\partial z})\ G(t,z)\Big|_{z=1} = \sum_n n\, p_n^m;$$

$$\therefore\ \mu_1' = (z \frac{\partial}{\partial z})\ G(t,z)\Big|_{z=1} \quad . \tag{24}$$

Without loss of generality, we define the initial position m of the adatom as zero, so that the generating function in Eq. (12) assumes a simpler form:

$$G(t,z) = \exp\{[\beta(z^2+z^{-2})+\alpha(z+z^{-1})-2(\alpha+\beta)]t\} \quad . \tag{25}$$

By substituting Eq. (25) into Eq(24) we can write the mean μ_1' as

$$\mu_1' = z(\frac{\partial}{\partial z})\ \exp\{[\beta(z^2+z^{-2})+\alpha(z+z^{-1})-2(\alpha+\beta)]t\}\Big|_{z=1}$$

$$= z\{[\beta(2z-2z^{-3})+\alpha(1-z^{-2})]t\}\ \exp\{[\beta(z^2+z^{-2})+\alpha(z+z^{-1})-2(\alpha+\beta)]t\}\Big|_{z=1}$$

$$= 1\{[\beta(2-2)+\alpha(1-1)]t\}\ \exp\{[\beta(1+1)+\alpha(1+1)\ -2(\alpha+\beta)]t\} = 0 \quad . \tag{26}$$

Just as expected from symmetry, μ_1' vanishes.

Any r-th moment can be found by the same route that lead to Eq. (24). Notice that

$$(z \frac{\partial}{\partial z})^r \sum_n z^n p_n^m = \sum_n n^r z^n p_n^m . \tag{27}$$

Evaluating Eq. (27) at $z = 1$ leads to the well known relation

$$(z \frac{\partial}{\partial z})^r \; G(t,z)\Big|_{z=1} = \sum_n n^r p_n^m \tag{28}$$

or

$$\mu_r' = (z \frac{\partial}{\partial z})^r \; G(t,z)\Big|_{z=1} . \tag{29}$$

We now have accessible any r-th moment of the adatom displacements occurring during a random walk lasting t seconds. The derivation of moments via Eq. (29) is conceptually simple; the actual calculations of higher moments are tedious and are therefore reserved for Appendix A.

Knowing the moments of the adatom displacements as a function of the jump rates α and β, we are ready for the problem of finding α and β in terms of the moments. In Appendix A, Eqs. (25) and (29) are used to derive the first two non-zero moments

$$\mu_2' = 2(4\beta + \alpha)t \tag{30a}$$

$$\mu_4' = 7\mu_2' + 3(\mu_2')^2 - 12(2\beta + \alpha)\ t. \tag{30b}$$

For the case where no double jumps occur and so $\beta = 0$, the second moment is

$$\mu_2' = 2\alpha t , \tag{31}$$

just as we would suspect from Eq. (3) for $\ell = 1$. Equations (30a) and (30b) are linearly independent; hence α and β can be expressed, in terms of μ_2' and μ_4', as

$$\alpha t = \frac{1}{6}\,[4\mu_2' + 3(\mu_2')^2 - \mu_4'] \tag{32a}$$

$$\beta t = \frac{1}{24}\,[\mu_4' - 3(\mu_2')^2 - \mu_2'] \quad . \tag{32b}$$

We recall from Eq. (21) that $\mu_r = \mu_r'$, so that αt and βt can be found in terms of moments about the mean as well as about zero.

C. Moments and Probability Densities

From Eq. (16) it is obvious that the probability density $p_n^m(t)$ for a random walk involving double and single jumps is uniquely characterized by the two jump rates β and α, and by the diffusion time t. We can reduce the number of parameters necessary to specify the distribution by representing $p_n^m(t)$ as a function of the second moment μ_2 and the ratio β/α. Equation (30a) gives the second moment in terms of α, β, and t, as

$$\mu_2 = 8\beta t + 2\alpha t \ . \tag{33}$$

We can find $2\beta t$ and $2\alpha t$ in terms of μ_2 and β/α from Eq. (33):

$$2\alpha t = \frac{\mu_2}{(1 + 4\beta/\alpha)} \tag{34a}$$

$$2\beta t = \frac{\mu_2}{(4 + \alpha/\beta)} = \frac{\mu_2\,\beta/\alpha}{(1 + 4\beta/\alpha)} \quad . \tag{34b}$$

Also,

$$(2\alpha t + 2\beta t) = \mu_2\,\frac{(1 + \beta/\alpha)}{(1 + 4\beta/\alpha)} \quad . \tag{34c}$$

Substituting Eqs. (34a), (34b), and (34c) into Eq. (16) for the probability density $p_n^m(t)$ yields this quantity as a function of μ_2 and β/α :

$$p_n^m(\mu_2, \beta/\alpha) =$$

$$\exp\left[-\mu_2\,\frac{(1+\beta/\alpha)}{(1+4\beta/\alpha)}\right] \sum_k I_k\!\left(\frac{\mu_2\,\beta/\alpha}{1+4\beta/\alpha}\right) I_{(n-m)-2k}\!\left(\frac{\mu_2}{1+4\beta/\alpha}\right) \quad . \tag{35}$$

In Appendix D is listed the FORTRAN program PPLOT [8] which calculates and plots the probability p_n^o as a function of lattice position n for various values of μ_2 and β/α. In Fig. 1 we show the behavior of an adatom executing a one-dimensional random walk. The distribution of distances for an adatom only allowed to make single jumps is compared with the distribution in which the adatom can make both double and single jumps as well as that in which only double jumps are allowed. As we vary the second moment from 10. to 1., the distribution where only double jumps are allowed begins to resemble that for single jumps more closely; the mixed distribution, for which $\beta/\alpha = 1.$, seems to become less like the distribution for single jumps. This is the sort of trend that we are looking for. In order to do an experiment aimed at detecting double jumps there must be differences between the distributions for different jump rates β/α. The trends in Fig. 1 suggest that the diffusion experiment should be done under conditions such that the second moment of the displacement distribution is much less than 10.0. Figure 1 also indicates that the second moment should be larger than .1; at this value all three distributions look very much the same, as little diffusion has occurred for any of the three examples.

In Fig. 2 we see how the probability distribution p_n^o calculated by PPLOT compares with available data. The experimental distance distribution is taken from Stolt's observations on one-dimensional diffusion of Re atoms over W(211) [4]. These observations were not made with the intention of looking for double jumps, so it is not surprising that the data are inadequate to show whether or not adatoms make occasional double jumps. The experiment that can answer this question will have to be planned specifically for the purpose of detecting such double jumps.

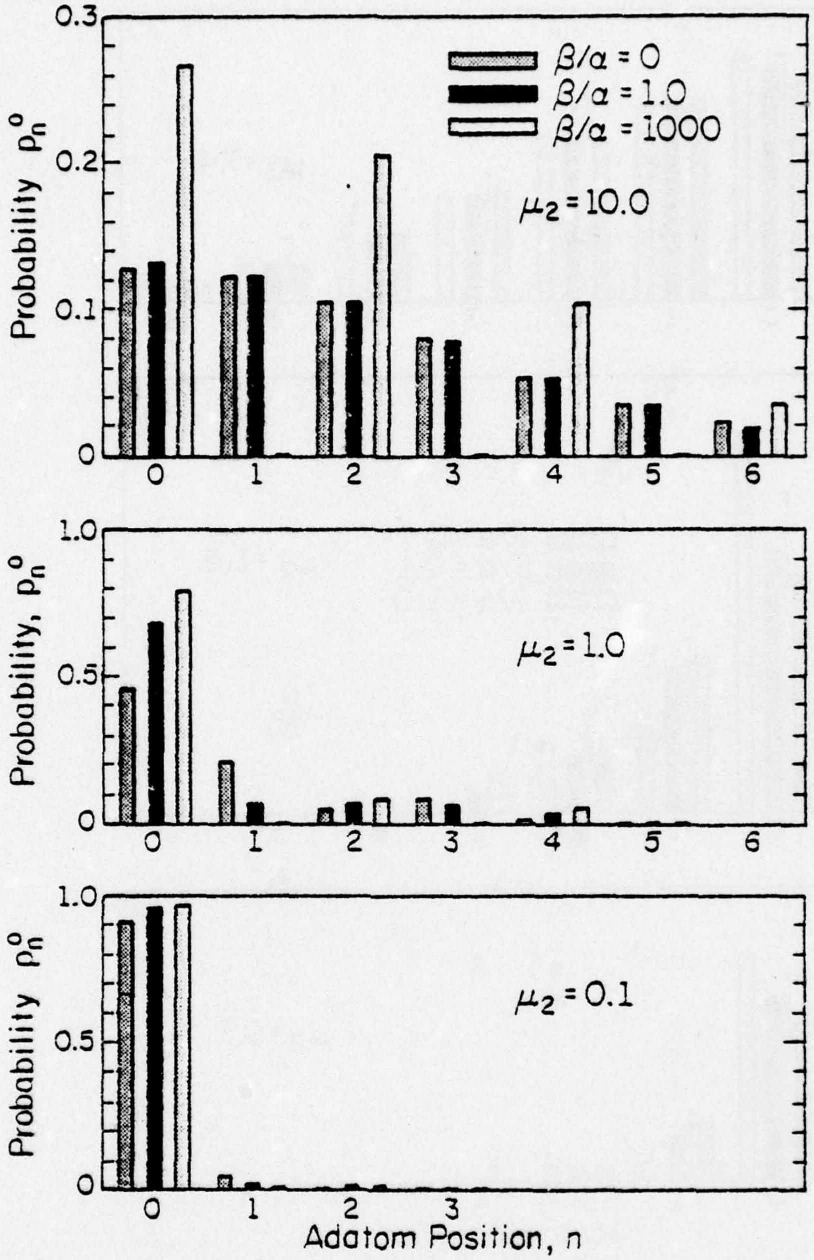

Figure 1. Distribution of distances covered during 1-dimensional diffusion of adatoms for different jump ratios β/α.

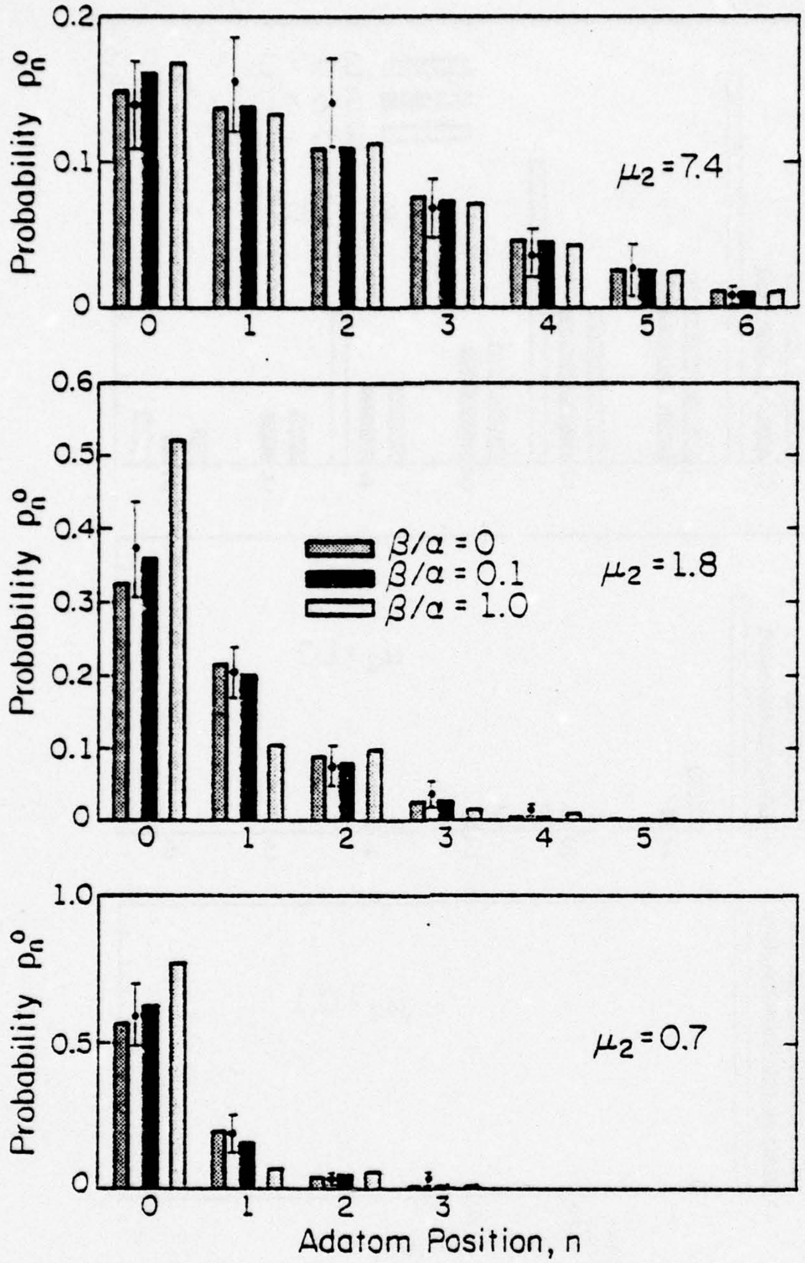

Figure 2. Distribution of distances covered during 1-dimensional diffusion of Re adatoms on W(211). Data points indicate experimental results of Stolt; bar graphs represent calculated probabilities.

II. PROBLEMS IN THE DETERMINATION OF JUMP RATES

A. Estimating Jump Rates from Diffusion Data

The problem now is to determine, by experiment, the values of the jump rates α and β for single and double jumps. From Eqs. (32a), (32b), and (21), we know that

$$\alpha t = \frac{1}{6}\,[4\mu_2 + 3(\mu_2)^2 - \mu_4] \tag{36a}$$

$$\beta t = \frac{1}{24}\,[\mu_4 - 3(\mu_2)^2 - \mu_2] \quad . \tag{36b}$$

The moments entering here are defined by Eq. (20b) as

$$\mu_r = \lim_{M\to\infty} \frac{1}{M} \sum_{i=1}^{M} (x_i - \mu_1')^r \ , \tag{37}$$

where x_i is the i-th observed adatom displacement and μ_1' is the mean of the displacements.

The moments μ_4 and μ_2 in Eqs. (36) are quantities established from an infinite number of observations. Such an infinitely large set of observations is called a population or parent population; quantities such as μ_4 and μ_2 that are derived from a population are referred to as population values. Specifically, μ_4 and μ_2 belong to a class of population values called parent moments. In order for μ_4 and μ_2 to be of any use to us, we must learn how to estimate them from a finite number of observations. Given a finite sample of observations taken from the parent population, we can generate statistics. A statistic is defined as any parameter generated by a finite number of observations; for each population parameter there is usually a corresponding statistic. The statistic that corresponds to a parent moment is called a sample moment. The r-th sample moment about

zero, m'_r, is defined as

$$m'_r \equiv \frac{1}{M} \sum_{i=1}^{M} (x_i)^r \ . \tag{38}$$

The r-th sample moment about the mean is defined as

$$m_r \equiv \frac{1}{M} \sum_{i=1}^{M} (x_i - m'_1)^r \ . \tag{39}$$

The statistic that corresponds to the second parent moment about the mean, μ_2, is the sample moment about the mean, m_2. From the definitions of μ_2 and m_2, we see that m_2 is a crude estimate of μ_2. If m_2 were an unbiased estimate of μ_2, the average or expectation value of m_2 would be equal to μ_2. This, however, is not the case. In Appendix B we find that the expectation value of m_2, $\langle m_2 \rangle$ is actually

$$\langle m_2 \rangle = \frac{M-1}{M} \mu_2 \ . \tag{40}$$

A better estimate of μ_2 is then

$$\hat{\mu}_2 = \frac{M}{M-1} m_2 \ . \tag{41}$$

By definition, $\hat{\mu}_2$ is the unbiased estimator of μ_2. In general, the statistic $\hat{\delta}$ is the unbiased estimator of the population value δ if and only if [9]

$$\langle \hat{\delta} \rangle = \delta \ . \tag{42}$$

Not all expectation values are quite as simple as $\hat{\mu}_2$. For example, the expectation value of the fourth parent moment about the mean is

$$\hat{\mu}_4 = m_4 \left[1 + \frac{4}{(M-1)} + \frac{12}{(M-1)^{[2]}} + \frac{18}{(M-1)^{[3]}} \right] - 3m_2^2 \left[\frac{2M}{(M-1)^{[2]}} + \frac{3M}{(M-1)^{[3]}} \right] \tag{43}$$

where M is the number of observations and

$$M^{[\rho]} \equiv (M-1)(M-2)\ldots(M-\rho+1) \quad . \tag{44}$$

The formal procedure for finding unbiased estimators and expectation values is left to Appendix B. Here, we are only interested in giving the motivation for such formal techniques. In Appendix C we employ these techniques to find the expectation values of αt and βt as given by Eqs. (C8a) and (C8b):

$$\hat{\alpha t} = R_\alpha m_2 + S_\alpha m_2^2 + T_\alpha m_4 \tag{45a}$$

$$\hat{\beta t} = R_\beta m_2 + S_\beta m_2^2 + T_\beta m_4 \; . \tag{45b}$$

The coefficients on the right hand side, according to Eqs. (C9) and (C10), are

$$R_\alpha = \frac{2}{3} \; \frac{M}{(M-1)} \tag{46a}$$

$$S_\alpha = \frac{M}{2}\left(\frac{1}{(M-1)} + \frac{4}{(M-1)^{[2]}} + \frac{6}{(M-1)^{[3]}}\right) \tag{46b}$$

$$T_\alpha = -\frac{1}{6}\left(1 + \frac{7}{(M-1)} + \frac{24}{(M-1)^{[2]}} + \frac{36}{(M-1)^{[3]}}\right) \tag{46c}$$

$$R_\beta = -\frac{1}{24} \; \frac{M}{(M-1)} \tag{47a}$$

$$S_\beta = -\frac{M}{8}\left(\frac{1}{(M-1)} + \frac{4}{(M-1)^{[2]}} + \frac{6}{(M-1)^{[3]}}\right) \tag{47b}$$

$$T_\beta = \frac{1}{24}\left(1 + \frac{7}{(M-1)} + \frac{24}{(M-1)^{[2]}} + \frac{36}{(M-1)^{[3]}}\right) \quad . \tag{47a}$$

We can substitute Eqs. (46) and (47) into Eqs. (45a) and (45b) to obtain expressions for αt and βt. That is,

$$\hat{\alpha t} = \frac{2}{3}\frac{M}{(M-1)}m_2$$

$$+\frac{M}{2}\left(\frac{1}{(M-1)}+\frac{4}{(M-1)^{[2]}}+\frac{6}{(M-1)^{[3]}}\right)m_2^2$$

$$-\frac{1}{6}\left(1+\frac{7}{(M-1)}+\frac{24}{(M-1)^{[2]}}+\frac{36}{(M-1)^{[3]}}\right)m_4 \tag{48a}$$

$$\hat{\beta t} = -\frac{1}{24}m_2$$

$$-\frac{M}{8}\left(\frac{1}{(M-1)}+\frac{4}{(M-1)^{[2]}}+\frac{6}{(M-1)^{[3]}}\right)m_2^2$$

$$+\frac{1}{24}\left(1+\frac{7}{(M-1)}+\frac{24}{(M-1)^{[2]}}+\frac{36}{(M-1)^{[3]}}\right)m_4 \,. \tag{48b}$$

The diffusion time t can generally be determined with arbitrarily good accuracy. Then knowing t, $\hat{\alpha}t$, and $\hat{\beta}t$ gives us $\hat{\alpha}$ and $\hat{\beta}$ directly, as

$$\hat{\alpha} = \hat{\alpha t}/t \tag{49a}$$

$$\hat{\beta} = \hat{\beta t}/t \tag{49b}$$

We now know how to estimate the jump rates α and β from an hypothetical data set. This knowledge is of little value, however, unless we can also estimate the random error incurred in making the measurements. The next problem we therefore consider is that of finding a measure of the random errors inherent in an experiment.

B. Estimating the Random Errors

The magnitude of the random error in the random variable $\hat{\alpha}t$ is indicated by the variance, defined as

$$\mathrm{var}\,\hat{\alpha t} \equiv \left\langle (\hat{\alpha t} - \langle\hat{\alpha t}\rangle)^2\right\rangle \,. \tag{50}$$

According to the definition of an unbiased estimator as expressed in Eq. (42),

$$\langle \hat{\alpha t} \rangle = \alpha t \ .$$

Equation (50) can be reduced to the equivalent form

$$\begin{aligned} \text{var}\ \hat{\alpha t} &= \langle (\hat{\alpha t} - \alpha t)^2 \rangle \\ &= \langle (\hat{\alpha t})^2 - 2\alpha t\ \hat{\alpha t} + (\alpha t)^2 \rangle \ . \end{aligned}$$

The expectation value of a sum is equal to the sum of the expectation values for each term of the sum so that

$$\text{var}\ \hat{\alpha t} = \langle (\hat{\alpha t})^2 \rangle - \langle 2\alpha t\ \hat{\alpha t} \rangle + \langle (\alpha t)^2 \rangle \ .$$

Because αt is a population value,

$$\langle 2\alpha t\ \hat{\alpha t} \rangle = 2\alpha t\ \langle \hat{\alpha t} \rangle = 2(\alpha t)^2$$

and

$$\langle (\alpha t)^2 \rangle = (\alpha t)^2 \ .$$

The variance of αt is thus given by the well know relation

$$\text{var}\ \hat{\alpha t} = \langle (\hat{\alpha t})^2 \rangle - (\alpha t)^2 \ . \tag{51a}$$

Similarly, the variance of $\hat{\beta t}$ is

$$\text{var}\ \hat{\beta t} = \langle (\hat{\beta t})^2 \rangle - (\beta t)^2 \ . \tag{51b}$$

However, the variances according to Eqs. (51) are population values, and therefore cannot be determined from a finite experiment. The unbiased estimators of var $\hat{\alpha t}$ and var $\hat{\beta t}$ though are random variables that are accessible through a finite number of observations. Using the operator U to indicate that an unbiased estimator is being taken, we write the unbiased estimator of var $\hat{\alpha t}$ as

$$U(\text{var}\ \hat{\alpha t}) = U(\langle (\hat{\alpha t})^2 \rangle - (\hat{\alpha t})^2) \ . \tag{52}$$

The operator U acts linearly, so that

$$U(\mathrm{var}\ \widehat{\alpha t}) = U[\langle(\widehat{\alpha t})^2\rangle] - U[(\alpha t)^2] \ .$$

The unbiased estimator of the expectation value of a random variable is equal to the random variable itself and therefore

$$U[\langle(\widehat{\alpha t})^2\rangle] = (\widehat{\alpha t})^2 \ .$$

An equivalent expression for U(var αt) is then

$$U(\mathrm{var}\ \widehat{\alpha t}) = (\widehat{\alpha t})^2 - U[(\alpha t)^2] \ . \tag{53a}$$

Similarly, the unbiased estimator of the variance of βt is

$$U(\mathrm{var}\ \widehat{\beta t}) = (\widehat{\beta t})^2 - U[(\widehat{\beta t})^2] \ . \tag{53b}$$

The error in measuring t is negligible compared with the error in $\hat{\alpha}$ and $\hat{\beta}$. That is,

$$\frac{U[\mathrm{var}\ \hat{\alpha}]}{(\hat{\alpha})^2} \cong \frac{U[\mathrm{var}\ \widehat{\alpha t}]}{(\hat{\alpha}t)^2} \tag{54a}$$

$$\frac{U[\mathrm{var}\ \hat{\beta}]}{(\hat{\beta})^2} \cong \frac{U[\mathrm{var}\ \widehat{\beta t}]}{(\hat{\beta}t)^2} \ . \tag{54b}$$

Substituting Eqs. (45a) and (45b) into Eqs. (53a) and (53b) respectively, we arrive at

$$\begin{aligned} U[\mathrm{var}\ \widehat{\alpha t}] &= (R_\alpha m_2 + S_\alpha m_2^2 + T_\alpha m_4)^2 - U[(\alpha t)^2] \\ &= R_\alpha^2 m_2^2 + 2R_\alpha S_\alpha m_2^3 + 2R_\alpha T_\alpha m_4 m_2 + S_\alpha^2 m_2^4 \\ &\quad + 2S_\alpha T_\alpha m_4 m_2^2 + T_\alpha^2 m_4^2 - U[(\alpha t)^2] \end{aligned} \tag{55}$$

where the coefficients R_α, S_α, and T_α have already been defined by Eqs. (46a)-(46c). In Appendix C, we find that $U[(\alpha t)^2]$ can be expressed in terms of

parameters k_{22}, k_{42}, and k_{44}, known as k-statistics, as

$$U[(\alpha t)^2] = \frac{4}{9} k_{22} - \frac{2}{9} k_{42} + \frac{1}{36} k_{44}. \tag{56}$$

As shown in Appendix C,

$$k_{22} = m_2^2 M^2 \left(\frac{1}{M^{[2]}} + \frac{2}{M^{[3]}} + \frac{3}{M^{[4]}} \right) - m_4 M \left(\frac{1}{M^{[2]}} + \frac{4}{M^{[3]}} + \frac{6}{M^{[4]}} \right) \tag{57a}$$

$$\begin{aligned} k_{42} = {} & m_6 M \left(-\frac{1}{M^{[2]}} - \frac{16}{M^{[3]}} - \frac{114}{M^{[4]}} - \frac{432}{M^{[5]}} - \frac{720}{M^{[6]}} \right) \\ & + m_4 m_2 M^2 \left(\frac{1}{M^{[2]}} + \frac{14}{M^{[3]}} + \frac{87}{M^{[4]}} + \frac{324}{M^{[5]}} + \frac{540}{M^{[6]}} \right) \\ & + m_3^2 M^2 \left(\frac{4}{M^{[3]}} + \frac{38}{M^{[4]}} + \frac{144}{M^{[5]}} + \frac{240}{M^{[6]}} \right) \\ & + m_2^3 M^3 \left(-\frac{3}{M^{[3]}} - \frac{15}{M^{[4]}} - \frac{54}{M^{[5]}} - \frac{90}{M^{[6]}} \right) \end{aligned} \tag{57b}$$

$$\begin{aligned} k_{44} = {} & m_8 M \left(-\frac{1}{M^{[2]}} - \frac{28}{M^{[3]}} - \frac{438}{M^{[4]}} - \frac{4320}{M^{[5]}} - \frac{27360}{M^{[6]}} - \frac{103680}{M^{[7]}} - \frac{181440}{M^{[8]}} \right) \\ & + m_6 m_2 M^2 \left(\frac{12}{M^{[3]}} + \frac{256}{M^{[4]}} + \frac{2736}{M^{[5]}} + \frac{18000}{M^{[6]}} + \frac{69120}{M^{[7]}} + \frac{120960}{M^{[8]}} \right) \\ & + m_5 m_3 M^2 \left(\frac{8}{M^{[3]}} + \frac{208}{M^{[4]}} + \frac{2304}{M^{[5]}} + \frac{14592}{M^{[6]}} + \frac{55296}{M^{[7]}} + \frac{96768}{M^{[8]}} \right) \\ & + m_4^2 M^2 \left(\frac{1}{M^{[2]}} + \frac{14}{M^{[3]}} + \frac{131}{M^{[4]}} + \frac{1080}{M^{[5]}} + \frac{6840}{M^{[6]}} + \frac{25920}{M^{[7]}} + \frac{45360}{M^{[8]}} \right) \\ & + m_4 m_2^2 M^3 \left(-\frac{6}{M^{[3]}} - \frac{102}{M^{[4]}} - \frac{972}{M^{[5]}} - \frac{6660}{M^{[6]}} - \frac{25920}{M^{[7]}} - \frac{45360}{M^{[8]}} \right) \\ & + m_3^2 m_2 M^3 \left(-\frac{64}{M^{[4]}} - \frac{912}{M^{[5]}} - \frac{6000}{M^{[6]}} - \frac{23040}{M^{[7]}} - \frac{40320}{M^{[8]}} \right) \\ & + m_2^4 M^4 \left(\frac{9}{M^{[4]}} + \frac{72}{M^{[5]}} + \frac{540}{M^{[6]}} + \frac{2160}{M^{[7]}} + \frac{3780}{M^{[8]}} \right) . \end{aligned} \tag{57c}$$

By substituting Eq. (56) into Eq. (55), we can estimate the variance of $\hat{\alpha t}$ in terms of sample moments about the mean and the k-statistics. That is,

$$U[\mathrm{var}\ \hat{\alpha t}] = R_\alpha^2 m_2^2 + 2R_\alpha S_\alpha m_2^3 + 2R_\alpha T_\alpha m_4 m_2 + S_\alpha^2 m_2^4 + 2S_\alpha T_\alpha m_4 m_2^2 + T_\alpha^2 m_4^2 - \frac{4}{9} k_{22} + \frac{2}{9} k_{42} - \frac{1}{36} k_{44} \tag{58a}$$

The coefficients R_α, S_α, and T_α are given by Eqs. (46a), (46b), and (46c). Similarly, the variance of $\hat{\beta t}$ can be estimated by

$$U[\mathrm{var}\ \hat{\beta t}] = R_\beta^2 m_2^2 + 2R_\beta S_\beta m_2^3 + 2R_\beta T_\beta m_4 m_2 + S_\beta^2 m_2^4 + 2S_\beta T_\beta m_4 m_2^2 + T_\beta^2 m_4^2 - \frac{1}{576} k_{22} + \frac{1}{288} k_{42} - \frac{1}{576} k_{44} \tag{58b}$$

where R_β, S_β, and T_β are given by Eqs. (47a), (47b), and (47c). The details are available in Appendix C.

Equations (58), (57), and (54) allow us to estimate the variance of $\hat{\alpha}$ and $\hat{\beta}$ from a hypothetical data set, consisting of M observations of adatom positions. We do not yet know, however, what experimental conditions yield the smallest variances for $\hat{\alpha}$ and $\hat{\beta}$; nor do we know how many observations are needed to insure statistical errors small enough to make $\hat{\alpha}$ and $\hat{\beta}$ meaningful. These problems are addressed in the next section.

C. Experimental Conditions Minimizing Random Errors

To minimize the random error in determining unbiased estimators for the rates of single and double jumps, we consider the variance predicted for different combinations of the rates α and β. We can calculate these variances from Eqs. (51a) and (51b):

$$\text{var}\ \widehat{\alpha t} = \langle (\widehat{\alpha t})^2 \rangle - (\alpha t)^2$$

$$\text{var}\ \widehat{\beta t} = \langle (\widehat{\beta t})^2 \rangle - (\beta t)^2 \ .$$

The evaluation of $\langle (\widehat{\alpha t})^2 \rangle$ and $\langle (\widehat{\beta t})^2 \rangle$ requires techniques developed in Appendix B, and is detailed in Appendix C. It is convenient to express the variances of $\widehat{\alpha t}$ and $\widehat{\beta t}$ in terms of the cumulants κ_2, κ_4, κ_6, and κ_8 which are in turn defined in terms of the parent moments μ_2, μ_4, μ_6, and μ_8 in Eqs. (60a)-(60b). That is,

$$\begin{aligned} \text{var}\ \widehat{\alpha t} = \frac{1}{36} \Big\{ & \frac{\kappa_8}{M} + \frac{16\kappa_6\kappa_2}{(M-1)} + \frac{(M+33)}{(M-1)}\kappa_4^2 + \frac{72\,M}{(M-1)^{[2]}}\kappa_4\kappa_2^2 \\ & + \frac{24M(M+1)}{(M-1)^{[3]}}\kappa_2^4 - \frac{8\kappa_6}{M} - \frac{8(M+7)}{(M-1)}\kappa_4\kappa_2 \\ & + \frac{16}{M}\kappa_4 + \frac{16(M+1)}{(M-1)}\kappa_2^2 \Big\} - (\alpha t)^2 \end{aligned} \tag{59a}$$

$$\begin{aligned} \text{var}\ \widehat{\beta t} = \frac{1}{576} \Big\{ & \frac{\kappa_8}{M} + \frac{16\kappa_6\kappa_2}{(M-1)} + \frac{(M+33)}{(M-1)}\kappa_4^2 + \frac{72M}{(M-1)^{[2]}}\kappa_4\kappa_2^2 \\ & + \frac{24M(M+1)}{(M-1)^{[3]}}\kappa_2^4 - \frac{2\kappa_6}{M} - \frac{2(M+7)\kappa_4\kappa_2}{(M-1)} \\ & + \frac{\kappa_4}{M} + \frac{(M+1)}{(M-1)}\kappa_2^2 \Big\} - (\beta t)^2 \ . \end{aligned} \tag{59b}$$

The properties of cumulants required for this work are discussed in Appendix B. Cumulants are related in a simple way to parent moments. Thus,

$$\kappa_2 = \mu_2 \tag{60a}$$

$$\kappa_4 = \mu_4 - 3\mu_2^2 \tag{60b}$$

$$\varkappa_6 = \mu_6 - 15\mu_4\mu_2 + 30\mu_2^3 \tag{60c}$$

$$\varkappa_8 = \mu_8 - 28\mu_6\mu_2 - 35\mu_4^2 + 420\mu_4\mu_2^2 - 630\mu_2^4. \tag{60d}$$

Though the exact expressions for var $\hat{\alpha t}$ and var $\hat{\beta t}$ are very complex, the corresponding approximations, to first order in 1/M are fairly simple. In Section 4 of Appendix C, Eqs. (C20) and (C22), we show that these approximations are given by

$$\text{var } \hat{\alpha t} = \frac{1}{36M} (\mu_8 - 12\mu_6\mu_2 - 2\mu_4^2 - 18\mu_4\mu_2^2 + 171\mu_2^4 + 136\mu_4\mu_2$$
$$- 72\mu_2^3 - 8\mu_6 + 16\mu_4 - 32\mu_2^2) \tag{61a}$$

$$\text{var } \hat{\beta t} = \frac{1}{576M} (\mu_8 - 12\mu_6\mu_2 - 2\mu_4^2 + 54\mu_4\mu_2^2 - 45\mu_2^4 - 2\mu_6$$
$$+ 16\mu_4\mu_2 - 18\mu_2^3 + \mu_4 - 2\mu_2^2) . \tag{61b}$$

Both of these approximations are within 6% of the corresponding exact variances for any value of β/α ranging from 0 to 1000, as long as $M \geq 100$ and $\mu_2 \leq 10$.

We can find the parent moments in terms of α, β, and t from the generating function, using Eqs. (25) and (29). These tedious calculations are preformed in Appendix A and yield the following:

$$\mu_2 = 2(4\beta t + \alpha t) \tag{62a}$$

$$\mu_4 = 7\mu_2 + 3(\mu_2)^2 - 12(2\beta t + \alpha t) \tag{62b}$$

$$\mu_6 = 128\beta t + 2\alpha t + 60(4\beta t + \alpha t)^2 + 720\beta t(4\beta t + \alpha t)$$
$$+ 120(4\beta t + \alpha t)^3 \tag{62c}$$

$$\mu_8 = 512\beta t + 2\alpha t + 64{,}512\ (\beta t)^2 + 252(\alpha t)^2 + 12{,}096(\alpha t)(\beta t)$$
$$+ 20{,}160(4\beta t + \alpha t)^2 + 1680(4\beta + \alpha t)^3 + 1680(4\beta t + \alpha t)^4. \tag{62d}$$

The aim of all this is to find the random error inherent in estimates of the jump rates $\hat{\alpha}$ and $\hat{\beta}$. The variances of $\widehat{\alpha t}$ and $\widehat{\beta t}$ are given by Eqs. (59), (60), and (62). Inasmuch as the error in the diffusion time t is insignificant, the error in measuring $\hat{\alpha}$ and $\hat{\beta}$ is identical to that of $\widehat{\alpha t}$ and $\widehat{\beta t}$; that is,

$$\frac{\text{var } \hat{\alpha}}{(\hat{\alpha})^2} = \frac{\text{var } \widehat{\alpha t}}{(\widehat{\alpha t})^2} \tag{63a}$$

$$\frac{\text{var } \hat{\beta}}{(\hat{\beta})^2} = \frac{\text{var } \widehat{\beta t}}{(\widehat{\beta t})^2} \quad . \tag{63b}$$

We recall from Eqs. (34a) and (34b), that αt and βt can be expressed in terms of μ_2 and β/α as

$$\alpha t = \frac{1}{2} \frac{\mu_2}{(1 + 4\beta/\alpha)} \tag{64a}$$

$$\beta t = \frac{1}{2} \frac{\mu_2 \; \beta/\alpha}{(1 + 4\beta/\alpha)} \quad . \tag{64b}$$

The relative error σ_α/α and σ_β/β in α and β is defined as

$$\frac{\sigma_\alpha}{\alpha} \equiv \left(\frac{\text{var } \hat{\alpha}}{\hat{\alpha}^2}\right)^{1/2} \tag{65a}$$

$$\frac{\sigma_\beta}{\beta} \equiv \left(\frac{\text{var } \hat{\beta}}{\hat{\beta}^2}\right)^{1/2} \quad . \tag{65b}$$

Equations (51), (59), (60), and (62)-(65) allow us to calculate exactly the relative error in α and β as a function of μ_2 for given values of M and β/α. These calculations were performed by the FORTRAN program KPLOT listed in Appendix D. Figure 3 shows σ_α/α and σ_β/β for β/α = .1 and .2 for M = 100, 1000, and 10,000. From Fig. 3 and Tables 1D-3D in Appendix D, we

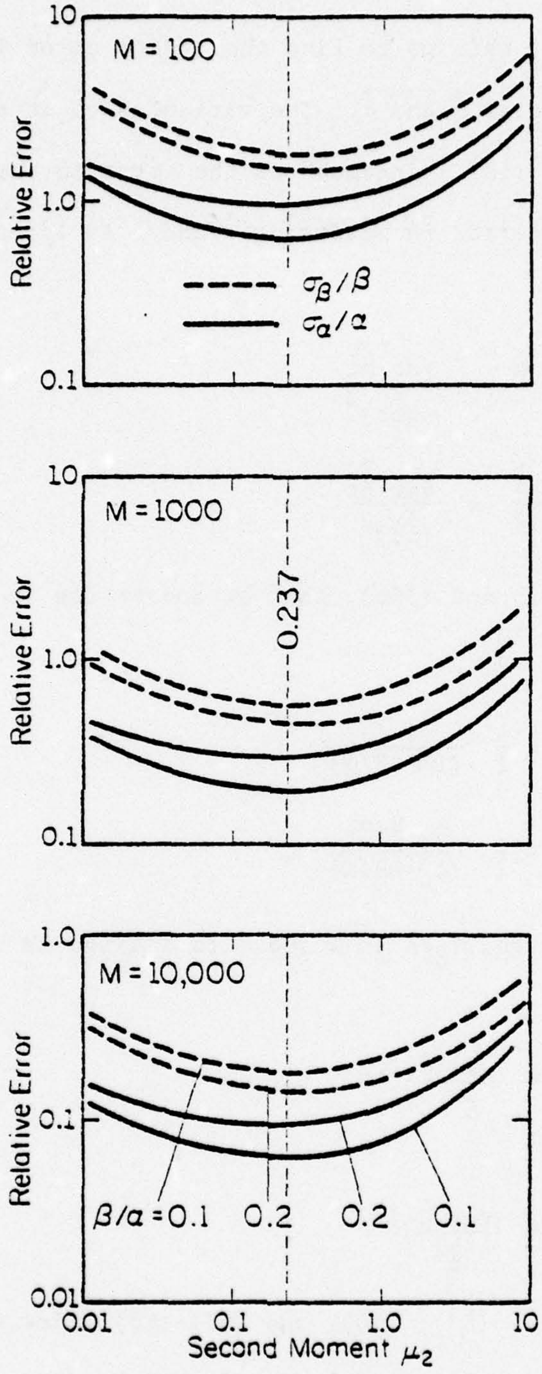

Figure 3. The relative error expected in the jump rate estimates $\hat{\alpha}$ and $\hat{\beta}$ as a function of the second moment μ_2.

see that σ_α/α and σ_β/β achieve their minimum values in the neighborhood of $\mu_2 = .237$ for the values of M and β/α given above. It is for this value of the second moment that measurements of the jump rates α and β are the most advantageous. Using the FORTRAN program MPLOT to calculate σ_α/α and σ_β/β as functions of M for $\mu_2 = .237$ and $\beta/\alpha = .1$ and .2, we find that only after a few thousand observations have been taken does the relative error drop to 40%, as shown in Fig. 4. For $M > 5000$, further increases in the number of observations have little effct. Precise determinations of the rate of double jumps therefore appear to be difficult; however, it should be possible in experiments of reasonable length to ascertain semiquantitatively if double jumps participate to any significant extent in the diffusion of single atoms over a surface.

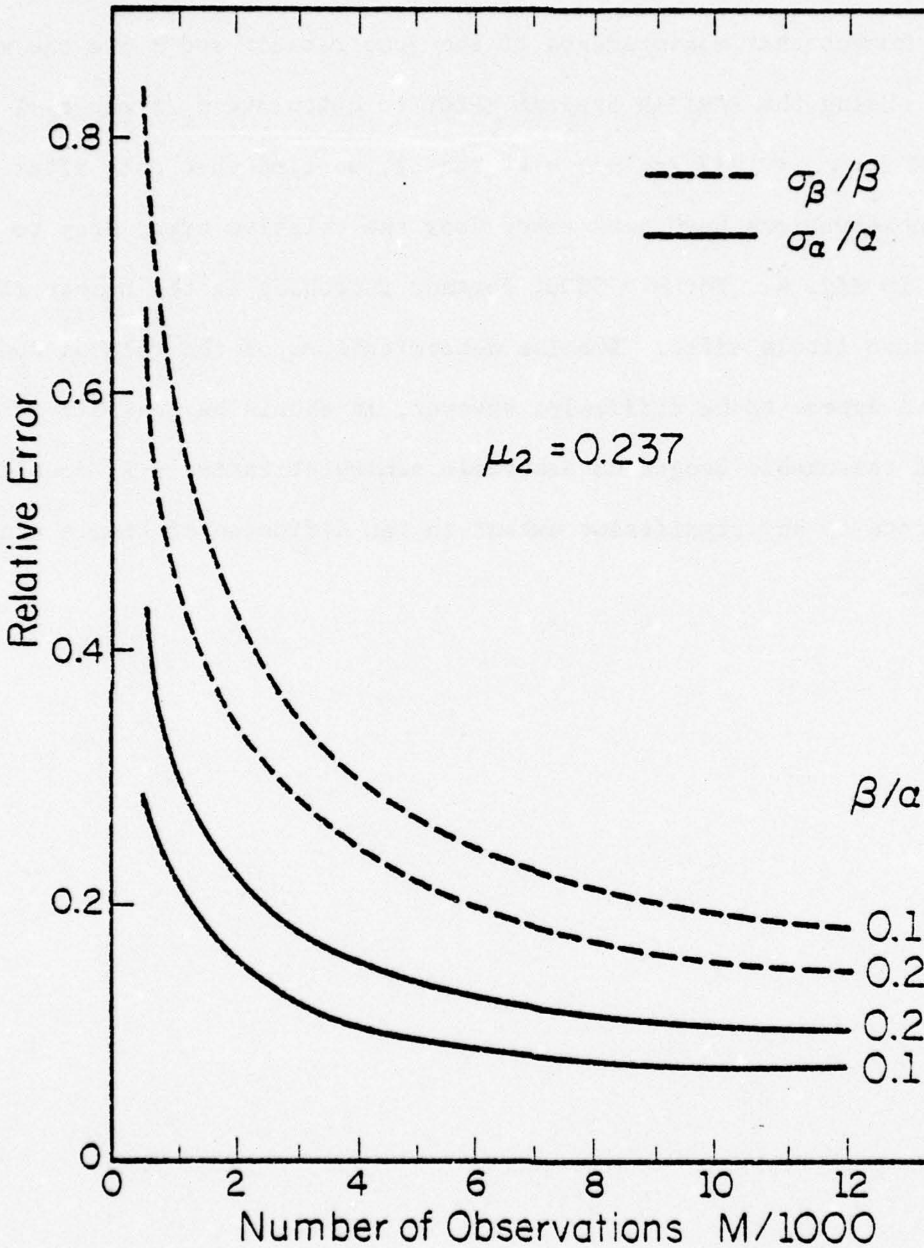

Figure 4. Relative error in jump rates as a function of M, the number of adatom diffusion intervals observed.

APPENDIX A

CALCULATION OF PARENT MOMENTS

1. General Approach

The aim of this appendix is to derive relations for the moments of the parent population of adatom displacements in terms of the jump rates α and β, and the diffusion interval t. Specifically, we are interested in finding the parent moments about the mean μ_2, μ_4, μ_6, and μ_8. Equations (21), (25), and (29) give us an algorithm for deriving the k-th parent moment about the mean μ_k

$$\mu_k = (z \frac{\partial}{\partial z})^k \, G(t,z) \Big|_{z=1} \quad . \tag{A1}$$

where

$$G(t,z) \equiv \exp\{[\beta(z^2 + z^{-2}) + \alpha(z + z^{-1}) - 2(\alpha + \beta)]t\} \ , \tag{A2}$$

or equivalently

$$\mu_k = \Gamma_k(t,1) \tag{A3}$$

where

$$\Gamma_k(t,z) \equiv (z \frac{\partial}{\partial z})^k G(t,z) \quad . \tag{A4}$$

Though the calculations for μ_2 and μ_4 are easy enough to perform, finding μ_6 and μ_8 requires a bit of forethought and careful bookkeeping. In order to facilitate the bookkeeping, we introduce the definitions

$$\dot{G} = \frac{\partial}{\partial z} G(t,z) \tag{A5a}$$

$$\ddot{G} = (\frac{\partial}{\partial z})^2 \, G(t,z) \tag{A5b}$$

$$G^{(k)} = (\frac{\partial}{\partial z})^k \, G(t,z) \tag{A5c}$$

$$F \equiv F(t,z) \equiv [\beta(z^2 + z^{-2}) + \alpha(z + z^{-1}) - 2(\alpha + \beta)]t \tag{A6}$$

$$\dot{F} = \frac{\partial}{\partial z} F(t,z) \tag{A7a}$$

$$\ddot{F} = (\frac{\partial}{\partial z})^2 F(t,z) \tag{A7b}$$

$$F^{(k)} = (\frac{\partial}{\partial z})^k F(t,z) \quad . \tag{A7c}$$

The procedures for utilizing Eqs. (A2)-(A7) to find μ_2, μ_4, μ_6, and μ_8 are outlined in the next section.

2. Outline for Moment Calculations

a. Find $\Gamma(t,z)$ through $\Gamma_8(t,z)$ in terms of $\dot{G}(t,z)$ and $G^{(8)}(t,z)$ using the recursion relation $\Gamma_{k+1}(t,z) = (z \frac{\partial}{\partial z}) \Gamma_k(t,z)$.

b. Find $\dot{G}(t,z)$ through $G^{(8)}(t,z)$ in terms of $\dot{F}(t,z)$ through $F^{(8)}(t,z)$ using the recursion relation $G^{(k+1)}(t,z) = (\partial/\partial z)G^{(k)}(t,z)$.

c. Find $\dot{F}(t,z)$ through $F^{(8)}(t,z)$ in terms of t, z, α, and β using the recursion relation $F^{(k+1)}(t,z) = (\partial/\partial z)F^{(k)}(t,z)$.

d. Evaluate $\dot{F}(t,1)$ through $F^{(8)}(t,1)$ in terms of α, β, and t.

e. Evaluate $\dot{G}(t,1)$ through $G^{(8)}(t,1)$ in terms of $\dot{F}(t,1)$ through $F^{(8)}(t,1)$.

f. Evaluate $\Gamma_k(t,1)$ for $k = 2,4,6$, and 8 first in terms of $\dot{F}(t,1)$ through $F^{(8)}(t,1)$ and then in terms of α, β, and t.

g. Keeping in mind that $\mu_k = \Gamma_k(t,1)$, find μ_2, μ_4, μ_6, and μ_8 in terms of α, β, and t.

3. Determination of $\Gamma_1(t,z)$ through $\Gamma_8(t,z)$

We use equation (A4) to generate the following recursion relation

$$\Gamma_{k+1}(t,z) = (z \frac{\partial}{\partial z}) \Gamma_k(t,z) \quad . \tag{A8}$$

This recursion formula will be used to find $\Gamma_1(t,z)$ through $\Gamma_8(t,z)$ in terms of $\dot{G}(t,z)$ through $G^{(8)}(t,z)$. For the purposes of these calculations we introduce the symbols

$$G^{(k)} \equiv G^{(k)}(t,z) \tag{A9a}$$

$$\Gamma_k \equiv \Gamma_k(t,z) \ . \tag{A9b}$$

Using these, we now write the Γ_k's as

$$\Gamma_1 = (z \frac{\partial}{\partial z}) G = z\dot{G} \tag{A10a}$$

$$\begin{aligned} \Gamma_2 &= (z \frac{\partial}{\partial z}) \Gamma_1 = (z \frac{\partial}{\partial z}) (z\dot{G}) \\ &= z(\dot{G} + z\ddot{G}) \\ &= z\dot{G} + z^2\ddot{G} \end{aligned} \tag{A10b}$$

$$\begin{aligned} \Gamma_3 &= (z \frac{\partial}{\partial z}) (z\dot{G} + z^2\ddot{G}) \\ &= z\dot{G} + z^2\ddot{G} + 2z^2\ddot{G} + z^3G^{(3)} \\ &= z\dot{G} + 3z^2\ddot{G} + z^3G^{(3)} \end{aligned} \tag{A10c}$$

$$\begin{aligned} \Gamma_4 &= (z \frac{\partial}{\partial z}) (z\dot{G} + 3z^2\ddot{G} + z^3G^{(3)}) \\ &= (z\dot{G} + z^2\ddot{G}) + (6z^2\ddot{G} + 3z^3G^{(3)}) \\ &\quad + (3z^3G^{(3)} + z^4G^{(4)}) \\ &= z\dot{G} + 7z^2\ddot{G} + 6z^3G^{(3)} + z^4G^{(4)} \end{aligned} \tag{A10d}$$

$$\Gamma_5 = (z\frac{\partial}{\partial z})[z\dot{G} + 7z^2\ddot{G} + 6z^3G^{(3)} + z^4G^{(4)}]$$
$$= (z\dot{G} + z^2\ddot{G}) + 7(2z^2\ddot{G} + z^3G^{(3)})$$
$$+ 6(3z^3G^{(3)} + z^4G^{(4)}) + (4z^4G^{(4)} + z^5G^{(5)})$$
$$= z\dot{G} + 15z^2\ddot{G} + 25z^3G^{(3)} + 10z^4G^{(4)} + z^5G^{(5)} \tag{A10e}$$

$$\Gamma_6 = (z\frac{\partial}{\partial z})(z\dot{G} + 15z^2\ddot{G} + 25z^3G^{(3)} + 10z^4G^{(4)} + z^5G^{(5)})$$
$$= (z\dot{G} + z^2\ddot{G}) + 15(2z^2\ddot{G} + z^3G^{(3)})$$
$$+ 25(3z^3G^{(3)} + z^4G^{(4)}) + 10(4z^4G^{(4)} + z^5G^{(5)})$$
$$+ (5z^5G^{(5)} + z^6G^{(6)})$$
$$= z\dot{G} + 31z^2\ddot{G} + 90z^3G^{(3)} + 65z^4G^{(4)}$$
$$+ 15z^5G^{(5)} + z^6G^{(6)} \tag{A10f}$$

$$\Gamma_7 = (z\frac{\partial}{\partial z})(z\dot{G} + 31z^2\ddot{G} + 90z^3G^{(3)} + 65z^4G^{(4)} + 15z^5G^{(5)} + z^6G^{(6)})$$
$$= (z\dot{G} + z^2\ddot{G}) + 31(2z^2\ddot{G} + z^3G^{(3)})$$
$$+ 90(3z^3G^{(3)} + z^4G^{(4)}) + 65(4z^4G^{(4)} + z^5G^{(5)})$$
$$+ 15(5z^5G^{(5)} + z^6G^{(6)}) + (6z^6G^{(6)} + z^7G^{(7)})$$
$$= z\dot{G} + 63z^2\ddot{G} + 301z^3G^{(3)}$$
$$+ 350z^4G^{(4)} + 140z^5G^{(5)} + 21z^6G^{(6)} + z^7G^{(7)} \tag{A10g}$$

$$\Gamma_8 = (z\frac{\partial}{\partial z})(z\dot{G} + 63z^2\ddot{G} + 301z^3G^{(3)}$$
$$+ 350z^4G^{(4)} + 140z^5G^{(5)} + 21z^6G^{(6)} + z^7G^{(7)})$$
$$= (z\dot{G} + z^2\ddot{G}) + 63(2z^2\ddot{G} + z^3G^{(3)})$$
$$+ 301(3z^3G^{(3)} + z^4G^{(4)}) + 350(4z^4G^{(4)} + z^5G^{(5)})$$
$$+ 140(5z^5G^{(5)} + z^6G^{(6)}) + 21(6z^6G^{(6)} + z^7G^{(7)})$$
$$+ (7z^7G^{(7)} + z^8G^{(8)})$$
$$= z\dot{G} + 127z^2\ddot{G} + 966z^3G^{(3)}$$
$$+ 1701z^4G^{(4)} + 1050z^5G^{(5)} + 266z^6G^{(6)}$$
$$+ 28z^7G^{(7)} + z^8G^{(8)} \quad . \qquad \text{(A10h)}$$

This completes the first stage of the derivation.

4. Relations for $\dot{G}(t,z)$ through $G^{(8)}(t,z)$

We use Eq. (A5c) to generate the recursion relation

$$G^{(k+1)}(t,z) = \frac{\partial}{\partial z} G^{(k)}(t,z) \quad . \qquad \text{(A11)}$$

This recursion formula will be used to find $\dot{G}(t,z)$ through $G^{(8)}$ in terms of $\dot{F}(t,z)$ through $F^{(8)}(t,z)$. For the purpose of these calculations we simplify the symbols to read

$$F \equiv F(t,z) \qquad \text{(A12a)}$$
$$F^{(k)} \equiv F^{(k)}(t,z) \quad . \qquad \text{(A12b)}$$

Using Eqs. (A2), (A5c), and (A6), we can now write the $G^{(k)}$ functions as

$$G^{(k)} = (\frac{\partial}{\partial z})^k \exp(F) \quad . \qquad \text{(A13)}$$

The recursion relation given by Eq. (A11) implies that the first eight derivatives of $G(t,z)$ can be written in terms of the first eight derivatives of $F(t,z)$ as

$$\dot{G} = \frac{\partial}{\partial z}(\exp F) = \dot{F}\exp F \qquad \text{(A14a)}$$

$$\ddot{G} = \frac{\partial}{\partial z}(\dot{F}\exp F) = \ddot{F}\exp F + \dot{F}(\dot{F}\exp F)$$

$$\ddot{G} = \ddot{F}\exp F + (\dot{F})^2\exp F \qquad \text{(A14b)}$$

$$\begin{aligned}
G^{(3)} &= \frac{\partial}{\partial z}(\ddot{F}\exp F + (\dot{F})^2\exp F) \\
&= [F^{(3)}\exp F + \ddot{F}(\dot{F}\exp F)] \\
&\quad + [(2\dot{F}\ddot{F})\exp F + (\dot{F})^2(\dot{F}\exp F)] \\
&= F^{(3)}\exp F + \ddot{F}\dot{F}\exp F + 2\dot{F}\ddot{F}\exp F + (\dot{F})^3\exp F \\
&= F^{(3)}\exp F + 3\ddot{F}\dot{F}\exp F + (\dot{F})^3\exp F \qquad \text{(A14c)}
\end{aligned}$$

$$\begin{aligned}
G^{(4)} &= \frac{\partial}{\partial z}(F^{(3)}\exp F + 3\ddot{F}\dot{F}\exp F + (\dot{F})^3\exp F) \\
&= [F^{(4)}\exp F + F^{(3)}(\dot{F}\exp F)] \\
&\quad + 3[F^{(3)}\dot{F}\exp F + \ddot{F}\ddot{F}\exp F + \ddot{F}\dot{F}(\dot{F}\exp F)] \\
&\quad + [3(\dot{F})^2\ddot{F}\exp F + (\dot{F})^3(\dot{F}\exp F)] \\
&= F^{(4)}\exp F + F^{(3)}\dot{F}\exp F + 3F^{(3)}\dot{F}\exp F \\
&\quad + 3(\ddot{F})^2\exp F + 3\ddot{F}(\dot{F})^2\exp F + 3(\dot{F})^2\ddot{F}\exp F + (\dot{F})^4\exp F \\
&= (F^{(4)} + 4F^{(3)}\dot{F} + 3(\ddot{F})^2 + 6\ddot{F}(\dot{F})^2 + (\dot{F})^4)\exp F \qquad \text{(A14d)}
\end{aligned}$$

$$\begin{aligned}
G^{(5)} &= [F^{(5)} + 4(F^{(4)}\dot{F} + F^{(3)}\ddot{F}) + 3(2\ddot{F}F^{(3)}) \\
&\quad + 6(F^{(3)}(\dot{F})^2 + 2\dot{F}(\ddot{F})^2) + 4(\dot{F})^3\ddot{F}]\exp F \\
&\quad + [F^{(4)}\dot{F} + 4F^{(3)}(\dot{F})^2 + 3(\ddot{F})^2\dot{F} + 6\ddot{F}(\dot{F})^3 + (\dot{F})^5]\exp F \\
&= \{F^{(5)} + 4F^{(4)}\dot{F} + 4F^{(3)}\ddot{F} + 6\ddot{F}F^{(3)} + 6F^{(3)}(\dot{F})^2 \\
&\quad + 12\dot{F}(\ddot{F})^2 + 4(\dot{F})^3\ddot{F} + F^{(4)}\dot{F} + 4F^{(3)}(\dot{F})^2 \\
&\quad + 3(\ddot{F})^2\dot{F} + 6\ddot{F}(\dot{F})^3 + (\dot{F})^5\}\exp F
\end{aligned}$$

$$= \{F^{(5)} + 5F^{(4)}\dot{F} + 10F^{(3)}\ddot{F} + 10F^{(3)}(\dot{F})^2$$

$$+ 15(\ddot{F})^2\dot{F} + 10\ddot{F}(\dot{F})^3 + (\dot{F})^5\} \exp F \qquad \text{(A14e)}$$

$$G^{(6)} = \{F^{(6)} + 5(F^{(5)}\dot{F} + F^{(4)}\ddot{F})$$

$$+ 10(F^{(4)}\ddot{F} + (F^{(3)})^2) + 10(F^{(4)}(\dot{F})^2 + 2F^{(3)}\ddot{F}\dot{F})$$

$$+ 15(2F^{(3)}\ddot{F}\dot{F} + (\ddot{F})^3) + 10(F^{(3)}(\dot{F})^3 + \ddot{F}3(\dot{F})^2\ddot{F}) + 5(\dot{F})^4\ddot{F}\} \exp F$$

$$+ \{F^{(5)}\dot{F} + 5F^{(4)}(\dot{F})^2 + 10F^{(3)}\ddot{F}\dot{F} + 10F^{(3)}(\dot{F})^3$$

$$+ 15(\ddot{F}\dot{F})^2 + 10\ddot{F}(\dot{F})^4 + (\dot{F})^6\} \exp F$$

$$= \{F^{(6)} + 5F^{(5)}\dot{F} + 5F^{(4)}\ddot{F} + 10F^{(4)}\ddot{F}$$

$$+ 10(F^{(3)})^2 + 10F^{(4)}(\dot{F})^2 + 20F^{(3)}\ddot{F}\dot{F} + 30F^{(3)}\ddot{F}\dot{F}$$

$$+ 15(\ddot{F})^3 + 10F^{(3)}(\dot{F})^3 + 30(\ddot{F}\dot{F})^2 + 5\ddot{F}(\dot{F})^4$$

$$+ F^{(5)}\dot{F} + 5F^{(4)}(\dot{F})^2 + 10F^{(3)}\ddot{F}\dot{F} + 10F^{(3)}(\dot{F})^3$$

$$+ 15(\ddot{F}\dot{F})^2 + 10\ddot{F}(\dot{F})^4 + (\dot{F})^6\} \exp F$$

$$= \{F^{(6)} + 6F^{(5)}\dot{F} + 15F^{(4)}\ddot{F} + 10(F^{(3)})^2 + 15F^{(4)}(\dot{F})^2$$

$$+ 60F^{(3)}\ddot{F}\dot{F} + 15(\ddot{F})^3 + 20F^{(3)}(\dot{F})^3 + 45(\ddot{F}\dot{F})^2$$

$$+ 15\ddot{F}(\dot{F})^4 + (\dot{F})^6\} \exp F \qquad \text{(A14f)}$$

$$G^{(7)} = \{F^{(7)} + 6(F^{(6)}\dot{F} + F^{(5)}\ddot{F})$$

$$+ 15(F^{(5)}\ddot{F} + F^{(4)}F^{(3)}) + 10(2F^{(3)}F^{(4)}) + 15(F^{(5)}(\dot{F})^2 + 2\ddot{F}\dot{F}F^{(4)})$$

$$+ 60(F^{(4)}\ddot{F}\dot{F} + F^{(3)}F^{(3)}\dot{F} + F^{(3)}\ddot{F}\ddot{F})$$

$$+ 15(3(\ddot{F})^2F^{(3)}) + 20(F^{(4)}(\dot{F})^3 + F^{(3)}3(\dot{F})^2\ddot{F})$$

$$+ 45(2)(\ddot{F}\dot{F})(F^{(3)}\dot{F} + (\ddot{F})^2) + 15(F^{(3)}(\dot{F})^4 + \ddot{F}4(\dot{F})^3\ddot{F})$$

$$+ 6(\dot{F})^5\ddot{F}\} \exp F$$

$$+ \{F^{(6)}\dot{F} + 6F^{(5)}(\dot{F})^2 + 15F^{(4)}\ddot{F}\dot{F} + 10(F^{(3)})^2\dot{F}$$

$$+ 15F^{(4)}(\dot{F})^3 + 60F^{(3)}\ddot{F}(\dot{F})^2 + 15(\ddot{F})^3\dot{F}$$

$$+ 20F^{(3)}(\dot{F})^4 + 45(\ddot{F})^2(\dot{F})^3 + 15\ddot{F}(\dot{F})^5 + (\dot{F})^7\} \exp F$$

$$= \{F^{(7)} + 6F^{(6)}\dot{F} + 6F^{(5)}\ddot{F} + 15F^{(5)}F + 15F^{(4)}F^{(3)} + 20F^{(4)}F^{(3)}$$
$$+ 15F^{(5)}(\dot{F})^2 + 30F^{(4)}\ddot{F}\dot{F} + 60F^{(4)}\ddot{F}\dot{F} + 60(F^{(3)})^2\dot{F} + 60F^{(3)}(\ddot{F})^2$$
$$+ 45(\ddot{F})^2F^{(3)} + 20F^{(4)}(\dot{F})^3 + 60F^{(3)}\ddot{F}(\dot{F})^2 + 90F^{(3)}\ddot{F}(\dot{F})^2 + 90(\ddot{F})^3\dot{F}$$
$$+ 15F^{(3)}(\dot{F})^4 + 60(\ddot{F})^2(\dot{F})^3 + 6(\dot{F})^5\ddot{F} + F^{(6)}\dot{F} + 6F^{(5)}(\dot{F})^2$$
$$+ 15F^{(4)}\ddot{F}\dot{F} + 10(F^{(3)})^2\dot{F} + 15F^{(4)}(\dot{F})^3 + 60F^{(3)}\ddot{F}(\dot{F})^2 + 15(\ddot{F})^3\dot{F}$$
$$+ 20F^{(3)}(\dot{F})^4 + 45(\ddot{F})^2(\dot{F})^3 + 15\ddot{F}(\dot{F})^5 + (\dot{F})^7 \} \exp F$$
$$= \{F^{(7)} + 7F^{(6)}\dot{F} + 21F^{(5)}\ddot{F} + 35F^{(4)}F^{(3)} + 21F^{(5)}(\dot{F})^2$$
$$+ 105F^{(4)}\ddot{F}\dot{F} + 70(F^{(3)})^2\dot{F} + 105F^{(3)}(\ddot{F})^2 + 35F^{(4)}(\dot{F})^3$$
$$+ 210F^{(3)}\ddot{F}(\dot{F})^2 + 105(\ddot{F})^3\dot{F} + 35F^{(3)}(\dot{F})^4 + 105(\ddot{F})^2(\dot{F})^3$$
$$+ 21\ddot{F}(\dot{F})^5 + (\dot{F})^7 \} \exp F. \qquad \text{(A14g)}$$

It is now convenient to define the function H_7, so that

$$G^{(7)} = H_7 \exp F .$$

Then

$$G^{(8)} = \dot{H}_7 \exp F + H_7\dot{F} \exp F$$
$$= \{F^{(8)} + 7(F^{(7)}\dot{F} + F^{(6)}\ddot{F}) + 21(F^{(6)}\ddot{F} + F^{(5)}F^{(3)}$$
$$+ 35(F^{(5)}F^{(3)} + F^{(4)}F^{(4)}) + 21(F^{(6)}(\dot{F})^2 + 2\dot{F}\ddot{F}F^{(5)})$$
$$+ 105(F^{(5)}\ddot{F}\dot{F} + F^{(4)}F^{(3)}\dot{F} + F^{(4)}(\ddot{F})^2)$$
$$+ 70(2F^{(3)}F^{(4)}\dot{F} + (F^{(3)})^2\ddot{F}) + 105(F^{(4)}(\ddot{F})^2 + F^{(3)}2\ddot{F}F^{(3)})$$
$$+ 35(F^{(5)}(\dot{F})^3 + F^{(4)}3(\dot{F})^2\ddot{F})$$
$$+ 210(F^{(3)}F^{(3)}(\dot{F})^2 + F^{(4)}\ddot{F}(\dot{F})^2 + F^{(3)}\ddot{F}2(\dot{F})\ddot{F})$$
$$+ 105(3(\ddot{F})^2F^{(3)}\dot{F} + (\ddot{F})^3\ddot{F}) + 35(F^{(4)}(\dot{F})^4 + F^{(3)}4(\dot{F})^3\ddot{F})$$
$$+ 105\ (2\ddot{F}F^{(3)}(\dot{F})^3 + 3(\dot{F})^2(\ddot{F})(\ddot{F})^2) + 21(F^{(3)}(\dot{F})^5 + 5(\dot{F})^4\ddot{F}\ddot{F})$$
$$+ 7(\dot{F})^6\ddot{F}\} \exp F + H_7\dot{F} \exp F \quad . \qquad \text{(A14h)}$$

5. Relations for $\dot{F}(t,z)$ through $F^{(8)}(t,z)$

In order to find $\dot{F}(t,z)$ through $F^{(8)}(t,z)$ in terms of t, z, α, and β, we need only take the first eight derivatives of F(t,z). The function F(t,z) is defined by Eq. (A6) as

$$F(t,z) = [\beta(z^2+z^{-2})+\alpha(z+z^{-1}) - 2(\alpha+\beta)]t \ .$$

As a way of simplifying Eq. (A6) we define

$$A \equiv \alpha t \tag{A15a}$$

$$B \equiv \beta t \ . \tag{A15b}$$

These definitions result in a new expression for F(t,z):

$$F(t,z) = B[z^2+z^{-2}] + A[z+z^{-1}] - 2(A+B) \ . \tag{A16}$$

The first eight derivatives of F(t,z) with respect to z now are given by

$$\dot{F} = B[2z - 2z^{-3}] + A[1-z^{-2}] \tag{A17a}$$

$$\ddot{F} = B(2+6z^{-4}) + 2Az^{-3} \tag{A17b}$$

$$F^{(3)} = -24Bz^{-5} - 6Az^{-4}$$

$$= -6[4Bz^{-5} + Az^{-4}] \tag{A17c}$$

$$F^{(4)} = 24[5Bz^{-6} + Az^{-5}] \tag{A17d}$$

$$F^{(5)} = -120[6Bz^{-7} + Az^{-6}] \tag{A17e}$$

$$F^{(6)} = 720[7Bz^{-8} + Az^{-7}] \tag{A17f}$$

$$F^{(7)} = -5040[8Bz^{-9} + Az^{-8}] \tag{A17g}$$

$$F^{(8)} = 40,320[9Bz^{-10} + Az^{-9}] \ . \tag{A17h}$$

6. Evaluating $\dot{F}(t,z)$ through $F^{(8)}(t,z)$ at $z = 1$

Sections 3 through 6 give us all of the information necessary to find $\Gamma_1(t,z)$ through $\Gamma_8(t,z)$ in terms of t, z, α, and β. In order to find μ_2, μ_4, μ_6, and μ_8 in terms of t, α, and β; we only need to find $\Gamma_2(t,z)$, $\Gamma_4(t,z)$, $\Gamma_6(t,z)$, and $\Gamma_8(t,z)$ at $z=1$. Because all the Γ_k's are in terms of the $G^{(k)}$'s, and all the $G^{(k)}$'s are in terms of the $F^{(k)}$'s, the $F^{(k)}$'s must first be evaluated at $z=1$.

Substituting $z=1$ in Eqs. (A17a)-(A17h) and (A16), we find that

$$F(t,1) = B\cdot 2 + A\cdot 2 - 2(A + B) = 0 \tag{A18}$$

$$\dot{F}(t,1) = B(2-2) + A(1-1) = 0 \tag{A19a}$$

$$\ddot{F}(t,1) = B[2 + 6] + 2A = 8B + 2A \tag{A19b}$$

$$F^{(3)}(t,1) = -6[4B + A] \tag{A19c}$$

$$F^{(4)}(t,1) = 24[5B + A] \tag{A19d}$$

$$F^{(5)}(t,1) = -120[6B + A] \tag{A19e}$$

$$F^{(6)}(t,1) = 720[7B + A] \tag{A19f}$$

$$F^{(7)}(t,1) = -5040[8B + A] \tag{A19g}$$

$$F^{(8)}(t,1) = 40,320[9B + A] \quad . \tag{A19h}$$

7. Evaluating $\dot{G}(t,z)$ through $G^{(8)}(t,z)$ at $z = 1$

Rather than immediately expressing $\dot{G}(t,1)$ through $G^{(8)}(t,1)$ in terms of α, β, and t, we choose to first express these functions in terms of $\dot{F}(t,1)$ through $F^{(8)}(t,1)$. We find that Eqs. (A14a) through (A14h) are considerably simplified by making the substitutions $F(t,1) = 0$, $\dot{F}(t,1) = 0$, and $z=1$. That is,

$$G(t,1) = \exp F(t,1) = 1 \tag{A20}$$

$$\dot{G}(t,1) = \dot{F}(t,1) = 0 \tag{A21a}$$

$$\ddot{G}(t,1) = \ddot{F}(t,1) \tag{A21b}$$

$$G^{(3)}(t,1) = F^{(3)}(t,1) \tag{A21c}$$

$$G^{(4)} = F^{(4)} + 3(\ddot{F})^2 \tag{A21d}$$

$$G^{(5)} = F^{(5)} + 10F^{(3)}\ddot{F} \tag{A21e}$$

$$G^{(6)} = F^{(6)} + 15F^{(4)}\ddot{F} + 10(F^{(3)})^2 + 15(\ddot{F})^3 \tag{A21f}$$

$$G^{(7)} = F^{(7)} + 21F^{(5)}\ddot{F} + 35F^{(4)}F^{(3)} + 105F^{(3)}(\ddot{F})^2 \tag{A21g}$$

$$\begin{aligned} G^{(8)} &= F^{(8)} + 7F^{(6)}\ddot{F} + 21F^{(6)}\ddot{F} + 21F^{(5)}F^{(3)} + 35F^{(5)}F^{(3)} + 35(F^{(4)})^2 \\ &\quad + 105F^{(4)}(\ddot{F})^2 + 70(F^{(3)})^2\ddot{F} + 105F^{(4)}(\ddot{F})^2 + 210(F^{(3)})^2\ddot{F} + 105(\ddot{F})^4 \\ &= F^{(8)} + 28F^{(6)}\ddot{F} + 56F^{(5)}F^{(3)} + 35(F^{(4)})^2 \\ &\quad + 210F^{(4)}(\ddot{F})^2 + 280(F^{(3)})^2\ddot{F} + 105(\ddot{F})^4 \ . \end{aligned} \tag{A21h}$$

8. Evaluating $\Gamma_2(t,1)$, $\Gamma_4(t,1)$, $\Gamma_6(t,1)$, and $\Gamma_8(t,1)$

We can find $\Gamma_k(t,1)$ in terms of $\dot{F}(t,1)$ through $F^{(8)}(t,1)$ by substituting Eqs. (A21a) through (A21h) into Eqs. (A10a) through (A10h). The Γ_k's can then be found in terms of α, β, and t by using Eqs. (A15), (A18), and (A19) to evaluate F(t,z) and its first eight derivatives at $z = 1$. That is,

$$\Gamma_2(t,1) = \ddot{G} = \ddot{F} = 2A + 8B \tag{A22a}$$

$$\begin{aligned} \Gamma_4(t,1) &= \dot{G} + 7\ddot{G} + 6G^{(3)} + G^{(4)} \\ &= 0 + 7(\ddot{F}) + 6(F^{(3)}) + (F^{(4)} + 3(\ddot{F})^2) \\ &= 7\mu_2 + 6[-6(4B+A)] + 24(5B+A) + 3(\mu_2)^2 \\ &= 7\mu_2 - 144B - 36A + 120B + 24A + 3(\mu_2)^2 \\ &= 7\mu_2 + 3(\mu_2)^2 - 24B - 12A \end{aligned} \tag{A22b}$$

$$\begin{aligned}
\Gamma_6(t,1) &= \dot{G} + 31\ddot{G} + 90G^{(3)} + 65G^{(4)} + 15G^{(5)} + G^{(6)} \\
&= 0 + 31\ddot{F} + 90F^{(3)} + 65(F^{(4)} + 3(\ddot{F})^2) \\
&\quad + 15(F^{(5)} + 10F^{(3)}\ddot{F}) + (F^{(6)} + 15F^{(4)}\ddot{F} + 10(F^{(3)})^2 + 15(\ddot{F})^3) \\
&= 31\ddot{F} + 90F^{(3)} + 65F^{(4)} + 195(\ddot{F})^2 + 15F^{(5)} + 150F^{(3)}\ddot{F} \\
&\quad + F^{(6)} + 15F^{(4)}\ddot{F} + 10(F^{(3)})^2 + 15(\ddot{F})^3 \\
&= 31(8B+2A) + 90[-6(4B+A)] + 65[24(5B+A)] \\
&\quad + 195(8B+2A)^2 + 15[-120(6B+A)] + 150[-6(4B+A)(8B+2A)] \\
&\quad + 720(7B+A) + 15[24(5B+A)(8B+2A)] + 10[-6(4B+A)]^2 + 15(8B+2A)^3 \\
&= 62(4B+A) - 540(4B+A) + 1560(5B+A) + 780(4B+A)^2 \\
&\quad - 1800(6B+A) - 1800(4B+A)^2 + 720(7B+A) + 720(5B+A)(4B+A) \\
&\quad + 360(4B+A)^2 + 120(4B+A)^3 \\
&= 62(4B+A) - 540(4B+A) + 1560(5B+A) - 1800(6B+A) + 720(7B+A) \\
&\quad + 780(4B+A)^2 - 1800(4B+A)^2 + 360(4B+A)^2 + 720(5B+A)(4B+A) \\
&\quad + 120(4B+A)^3 \\
&= -478(4B+A) + (7800B + 1560A - 10800B - 1800A + 5040B + 720A) \\
&\quad - 660(4B+A)^2 + 720(5B+A)(4B+A) + 120(4B+A)^3 \\
&= -1912B - 478A + 2040B + 480A - 660(4B+A)^2 + 720(4B+A)^2 \\
&\quad + 720B(4B+A) + 120(4B+A)^3 \\
&= 128B + 2A + 60(4B+A)^2 + 720B(4B+A) + 120(4B+A)^3 \qquad \text{(A22c)}
\end{aligned}$$

$$\begin{aligned}
\Gamma_8(t,1) &= \dot{G} + 127\ddot{G} + 966G^{(3)} + 1701G^{(4)} + 1050G^{(5)} + 266G^{(6)} + 28G^{(7)} + G^{(8)} \\
&= 127\ddot{F} + 966F^{(3)} + 1701(F^{(4)} + 3(\ddot{F})^3) + 1050(F^{(5)} + 10F^{(3)}\ddot{F}) \\
&\quad + 266(F^{(6)} + 15F^{(4)}\ddot{F} + 10(F^{(3)})^2 + 15(\ddot{F})^3) \\
&\quad + 28(F^{(7)} + 21F^{(5)}\ddot{F} + 35F^{(4)}F^{(3)} + 105F^{(3)}(\ddot{F})^3) \\
&\quad + F^{(8)} + 28F^{(6)}\ddot{F} + 56F^{(5)}F^{(3)} + 35(F^{(4)})^2 \\
&\quad + 210F^{(4)}(\ddot{F})^2 + 280(F^{(3)})^2\ddot{F} + 105(\ddot{F})^4
\end{aligned}$$

$$= 127\ddot{F} + 966F^{(3)} + 1701F^{(4)} + 5103(\ddot{F})^2$$

$$+ 1050F^{(5)} + 10{,}500F^{(3)}\ddot{F}$$

$$+ 266F^{(6)} + 3990F^{(4)}\ddot{F} + 2660(F^{(3)})^2 + 3990(\ddot{F})^3$$

$$+ 28F^{(7)} + 588F^{(5)}\ddot{F} + 980F^{(4)}F^{(3)} + 2940F^{(3)}(\ddot{F})^2$$

$$+ F^{(8)} + 28F^{(6)}\ddot{F} + 56F^{(5)}F^{(3)} + 35(F^{(4)})^2$$

$$+ 210F^{(4)}(\ddot{F})^2 + 280(F^{(3)})^2\ddot{F} + 105(\ddot{F})^4$$

$$= 127[2(4B + A)] + 966[-6(4B + A)]$$

$$+ 1701[24(5B + A)] + 5103[2(4B + A)]^2$$

$$+ 1050[-120(6B + A)] + 10{,}500[-6(4B + A)][2(4B + A)]$$

$$+ 266[720(7B + A)] + 3990[24(5B + A)][2(4B + A)]$$

$$+ 2660[-6(4B + A)]^2 + 3990[2(4B + A)]^3$$

$$+ 28[-5040(8B + A)] + 588[-120(6B + A)][2(4B + A)]$$

$$+ 980[24(5B + A)][-6(4B + A)] + 2940[-6(4B + A)][2(4B + A)]^2$$

$$+ [40{,}320(9B + A)] + 28[720(7B + A)][2(4B + A)]$$

$$+ 56[-120(6B + A)][-6(4B + A)] + 35[24(5B + A)]^2$$

$$+ 210[24(5B + A)][2(4B + A)]^2 + 280[-6(4B + A)]^2[2(4B + A)]$$

$$+ 105[2(4B + A)]^4$$

$$= B[127(2)4 - 966(6)4 + 1701(24)5 - 1050(120)6 + 266(720)7$$

$$- 28(5040)8 + 40{,}320(9)] + A[127(2) - 966(6) + 1701(24)$$

$$- 1050(120) + 266(720) - 28(5040) + 40{,}320]$$

$$+ B^2[5103(4)(16) - 10{,}500(12)(16) + 3990(48)(20) + 2660(36)(16)$$

$$- 588(240)(24) - 980(144)(20) + 28(1440)(28) + 56(720)(24)$$

$$+ 35(24)^2(25)]$$

$$+ A^2[5103(4) - 10{,}500(12) + 3990(48)$$

$$+ 2660(36) - 588(240) - 980(144)$$

$$+ 28(1440) + 56(720) + 35(24)^2]$$

$$+ AB[5103(4)(8) - 10,500(12)(8) + 3990(48)(9)$$
$$+ 2660(36)(8) - 588(240)(10) - 980(144)(9)$$
$$+ 28(1440)(11) + 56(720)(10) + 35(24)^2(10)]$$
$$+ (4B+A)^3[3990(8) - 2940(24) + 280(72)]$$
$$+ 210(96)(5B+A)(4B+A)^2$$
$$+ 105(16)(4B+A)^4$$
$$= 512B + 2A$$
$$+ 64,512\, B^2 + 252A^2$$
$$+ 12,096AB - 18,480(4B+A)^3$$
$$+ 20,160(5B+A)(4B+A)^2 + 1680(4B+A)^4 \quad .$$

Note that

$$-18,480(4B+A)^3 + 20,160[(5B+A)(4B+A)^2]$$
$$= -18,480(4B+A)^3 + 20,160[B(4B+A)^2 + (4B+A)^3]$$
$$= 1680(4B+A)^3 + 20,160B(4B+A)^2 .$$

This makes it possible to write $\Gamma_8(t,1)$ as

$$\Gamma_8(t,1) = 512B+2A+64,512B^2+252A^2+12,096AB$$
$$+ 20,160B(4B+A)^2+1680(4B+A)^3+1680(4B+A)^4 . \qquad \text{(A22d)}$$

This completes the derivation of $\Gamma_2(t,1)$, $\Gamma_4(t,1)$, $\Gamma_6(t,1)$, and $\Gamma_{8'}(t,1)$.

9. The Parent Moments in Terms of α, β, and t

We know from Eq. (A3) that $\mu_k = \Gamma_k(t,1)$; Eqs. (A3), (A15), and (A22) therefore allow us to find the even moments of the parent population in terms of the jump rates α and β and the time interval t, as

$$\mu_2 = 2(4\beta + \alpha t) \qquad \text{(A23a)}$$

$$\mu_4 = 7\mu_2 + 3(\mu_2)^2 - 12(2\beta t + \alpha t) \qquad \text{(A23b)}$$

$$\mu_6 = 128\beta t + 2\alpha t + 60(4\beta t + \alpha t)^2 + 720\beta t(4\beta t + \alpha t) + 120(4\beta t + \alpha t)^3 \tag{A23c}$$

$$\mu_8 = 512\beta t + 2\alpha t + 64,512(\beta t)^2 + 252(\alpha t)^2 + 12,096(\alpha t)(\beta t) + 20,160(4\beta t + \alpha t)^2 + 1680(4\beta t + \alpha t)^3 + 1680(4\beta t + \alpha t)^4 \; . \tag{A23d}$$

This completes the derivation of the moments expressed in terms of the jump rates for single and double jumps.

APPENDIX B

UNBIASED ESTIMATORS OF MOMENTS ABOUT THE MEAN

This appendix is meant to serve as a tutorial for the statistical techniques employed in this thesis. The major source of this material is Kendall and Stuart's book on advanced statistics [9]. The reader is assumed to have a knowledge of statistics at the level of Bevington's book on data analysis [10]. Topics covered here include power sums, augmented symmetric functions, cumulants, and k-statistics.

1. The Second Moment

As an introduction to the statistical techniques used in finding the variances of the jump rates α and β, we will consider the problem of estimating the second parent moment about the mean μ_2, given a sample consisting of M observations. It is well known that the unbiased estimator of μ_2 is

$$\hat{\mu}_2 = \frac{M}{M-1} m_2 \ . \tag{B1}$$

Here m_2 is the second moment for a sample consisting of M observations. If Eq. (B1) correctly estimates μ_2, then Eq. (42) implies that the expectation value of $\hat{\mu}_2$ is μ_2. That is,

$$\langle \hat{\mu}_2 \rangle = \mu_2 \ . \tag{B2}$$

Because the number of observations M is not a random variable, we know that

$$\langle \hat{\mu}_2 \rangle = \frac{M}{M-1} \langle m_2 \rangle = \mu_2$$

or

$$\langle m_2 \rangle = \frac{M-1}{M} \mu_2 \ . \tag{B3}$$

Equation (B1) can be verified by finding the expectation value of m_2. From Eqs. (38) and (39) we find that m_2 can be expressed in terms of the M observations x_i comprising the sample as

$$m_2 = \frac{1}{M} \sum_{i=1}^{M} (x_i - \frac{1}{M} \sum_{j=1}^{M} x_j)^2 . \tag{B4}$$

Here and throughout this appendix, we will omit the bounds on the summation symbol and assume that every index is summed from 1 to M. Equation (B4) can then be written equivalently as

$$m_2 = \frac{1}{M} \Sigma(x_i - \Sigma x_j/M)^2 . \tag{B5}$$

We can reduce m_2 to a simpler form by expanding Eq. (B5):

$$\begin{aligned} m_2 &= \frac{1}{M} \Sigma[x_i^2 - 2x_i\Sigma x_j/M + (\Sigma x_j/M)^2] \\ &= \frac{1}{M} \Sigma x_i^2 - \frac{2}{M^2} (\Sigma x_i)(\Sigma x_j) + (\Sigma x_j/M)^2 \\ &= \frac{1}{M} \Sigma x_i^2 - \frac{1}{M^2} (\Sigma x_i)^2 . \end{aligned} \tag{B6}$$

Because the expectation value of a sum is the sum of the expectation values,

$$\begin{aligned} \langle m_2 \rangle &= \langle \frac{1}{M} \Sigma x_i^2 \rangle - \langle \frac{1}{M^2} (\Sigma x_i)^2 \rangle \\ &= \frac{1}{M} \Sigma \langle x_i^2 \rangle - \frac{1}{M^2} \langle (\Sigma x_i)^2 \rangle . \end{aligned} \tag{B7}$$

We already know that

$$\langle x_i^2 \rangle = \mu_2' ;$$

the first term of Eq. (B7) is therefore obvious. In order to write the second expression on the right in terms of parent moments, we must first

observe that

$$(\Sigma x_i)^2 = \Sigma x_i^2 + \sum_{i \neq j} x_i x_j \ . \tag{B8}$$

Because $i \neq j$ for each uncorrelated product $x_i x_j$, assigning M different values to i would leave only (M-1) values to be assigned to j. The second term of Eq. (B8) therefore consists of a sum over M(M-1) uncorrelated products $x_i x_j$. By substituting Eq. (B8) into Eq. (B7) we find that

$$\begin{aligned} \langle m_2 \rangle &= \frac{1}{M} \Sigma \langle x_i^2 \rangle - \frac{1}{M^2} \langle \Sigma x_i^2 + \sum_{i \neq j} x_i x_j \rangle \\ &= \mu_2' - \frac{1}{M^2} [M \langle x_i^2 \rangle + M(M-1) \langle x_i x_j \rangle] \\ &= \mu_2' - \frac{1}{M} \mu_2' - \frac{(M-1)}{M} \langle x_i x_j \rangle \ . \end{aligned} \tag{B9}$$

The expectation value of the product of statistically uncorrelated factors is the product of the expectation values of those factors. Therefore,

$$\langle x_i x_j \rangle = \langle x_i \rangle \langle x_j \rangle \tag{B10}$$

and

$$\begin{aligned} \langle m_2 \rangle &= \frac{(M-1)}{M} \mu_2' - \frac{(M-1)}{M} \langle x_i \rangle \langle x_j \rangle \\ &= \frac{(M-1)}{M} \mu_2' - \frac{(M-1)}{M} \mu_1' \mu_1' \\ &= \frac{(M-1)}{M} (\mu_2' - \mu_1'^2) \ . \end{aligned} \tag{B11}$$

From Eq. (20b) we know that

$$\begin{aligned} \mu_2 &= \langle (x_i - \mu_1')^2 \rangle \\ &= \langle x_i^2 - 2x_i \mu_1' + \mu_1'^2 \rangle \\ &= \langle x_i^2 \rangle - \langle 2x_i \mu_1' \rangle + \langle \mu_1'^2 \rangle \ . \end{aligned}$$

The parent mean μ_1' is not a statistic, so that

$$\mu_2 = \langle x_i \rangle^2 - 2\mu_1' \langle x_i \rangle + \mu_1'^2$$

$$= \mu_2' - 2\mu_1'\mu_1' + \mu_1'^2$$

$$= \mu_2' - \mu_1'^2 \quad . \tag{B12}$$

We substitute Eq. (B12) into Eq. (B11) and find that

$$\langle m_2 \rangle = \frac{(M-1)}{M} \mu_2 ,$$

which agrees with Eq. (B3). We have proven Eq. (B1), though not in the most elegant manner. In the next section, we introduce techniques that simplify such calculations.

2. Augmented Symmetric Functions and Power Sums

We noted that by writing m_2 in terms of Σx_i^2 and $\sum\limits_{i \neq j} x_i x_j$, we could easily find $\langle m_2 \rangle$ in terms of parent moments. From Eqs. (B6) and (B8), we know that

$$m_2 = \frac{1}{M} \Sigma x_i^2 - \frac{1}{M^2} (\Sigma x_i^2 + \sum_{i \neq j} x_i x_j)$$

$$= \frac{(M-1)}{M^2} \Sigma x_i^2 - \frac{1}{M^2} \sum_{i \neq j} x_i x_j \quad . \tag{B13}$$

The sums Σx_i^2 and $\sum\limits_{i \neq j} x_i x_j$ belong to a class of statistics known as augmented symmetric functions. In the notation associated with this class of statistics, these two sums are represented by

$$[2] = \Sigma x_i^2 \tag{B14a}$$

$$[1^2] = \sum_{i \neq j} x_i x_j \quad . \tag{B14b}$$

In general, augmented symmetric functions are defined as

$$[p_1 p_2 \ldots p_s] \equiv \Sigma\, x_i^{p_1} x_j^{p_2} \ldots x_v^{p_s} \quad . \tag{B15}$$

The indices i through v are summed from 1 to M, though in no term of the sum are any two or more of these indices allowed to have the same value. As an example of this notation, we will compute the augmented symmetric function [221] from the four element data set: $x_1 = -1$, $x_2 = 3$, $x_3 = -1$, and $x_4 = 0$. We can express [221] as

$$[221] = \Sigma\, x_i^2 x_j^2 x_k$$

where $i \neq j$, $j \neq k$, and $i \neq k$ for every term of the sum. The number of terms belonging to [221] is equal to the number of permutations of 4 objects taken 3 at a time. This number is

$$\frac{4!}{(4-3)!} = 4(4-1)\ldots(4-3+1) = 4 \cdot 3 \cdot 2 = 24.$$

These 24 permutations and the corresponding term of each is given in Table B1 below. There we find that [221] has a value of -30 for this data set.

There is a more elegant notation for expressing augmented symmetric functions than that shown in Eq. (B15). For example, we could write [221] as $[2^2 1]$ or [333 2222 11] as $[3^2 2^4 1^2]$. In general, augmented symmetric functions can be defined by this notation as

$$[p_1^{\lambda_1}\, p_2^{\lambda_2} \ldots p_s^{\lambda_s}] \equiv$$

$$\Sigma(x_a^{p_1} \ldots x_d^{p_1})(x_e^{p_2} \ldots x_h^{p_2}) \ldots (x_m^{p_s} \ldots x_r^{p_s}) \quad . \tag{B16}$$

where λ_i indicates the number of powers p_i in each term of the sum. No two or more of the indices a through r, as they are summed from 1 to M,

TABLE B1 - The augmented symmetric function [211] computed from the data set $\{-1, 3, -1, 0\}$.

i	j	k	x_i	x_j	x_k	$x_i^2 x_j^2 x_k$
1	2	3	-1	3	-1	-9
1	2	4	-1	3	0	0
1	3	2	-1	-1	3	3
1	3	4	-1	-1	0	0
1	4	2	-1	0	3	0
1	4	3	-1	0	-1	0
2	1	3	3	-1	-1	-9
2	1	4	3	-1	0	0
2	3	1	3	-1	-1	-9
2	3	4	3	-1	0	0
2	4	1	3	0	-1	0
2	4	3	3	0	-1	0
3	1	2	-1	-1	3	3
3	1	4	-1	-1	0	0
3	2	1	-1	3	-1	-9
3	2	4	-1	3	0	0
3	4	1	-1	0	-1	0
3	4	2	-1	0	3	0
4	1	2	0	-1	3	0
4	1	3	0	-1	-1	0
4	2	1	0	3	-1	0
4	2	3	0	3	-1	0
4	3	1	0	-1	-1	0
4	3	2	0	-1	3	0
						-30

may be equal for any one term of the sum. Specific examples of this notation are

$$[21^2] = \Sigma\, x_a^2 x_b x_c$$

$$[62^3 1] = \Sigma\, x_a^6 x_b^2 x_c^2 x_d^2 x_e$$

$$[7^2 2^3] = \Sigma\, x_a^7 x_b^7 x_c^2 x_d^2 x_e^2 \; .$$

Each term of $[p_1^{\lambda_1}\, p_2^{\lambda_2} \ldots p_s^{\lambda_s}]$ is a product of ρ factors where

$$\rho \equiv \lambda_1 + \lambda_2 + \ldots \lambda_s \; . \tag{B17}$$

Each term of $[p_1^{\lambda_1} p_2^{\lambda_2} \ldots p_s^{\lambda_s}]$ then corresponds to an element of the set of permutations generated by M objects taken ρ at a time. The number of such permutations and therefore the number of terms in $[p_1^{\lambda_1} p_2^{\lambda_2} \ldots p_s^{\lambda_s}]$ is

$$M^{[\rho]} \equiv M(M-1) \ldots (M-\rho+1) \; . \tag{B18}$$

It follows that any augmented symmetric function characterized by M observations and a given value of ρ can be expressed as a sum of $M^{[\rho]}$ terms. The expectation value of such an augmented symmetric function is

$$\langle [p_1^{\lambda_1} p_2^{\lambda_2} \ldots p_s^{\lambda_s}] \rangle$$

$$= \langle \Sigma (x_i^{p_1} \ldots x_j^{p_1})(x_q^{p_2} \ldots x_r^{p_2}) \ldots (x_u^{p_s} \ldots x_v^{p_s}) \rangle$$

$$= M^{[\rho]} \langle (x_1^{p_1} \ldots x_j^{p_1})(x_q^{p_2} \ldots x_r^{p_2}) \ldots (x_u^{p_s} \ldots x_v^{p_s}) \rangle \; .$$

Each of the ρ subfactors is statistically independent so that

$$\langle [p_1^{\lambda_1} p_2^{\lambda_2} \ldots p_s^{\lambda_s}] \rangle =$$

$$M^{[\rho]} (\langle x_i^{p_1} \rangle \ldots \langle x_j^{p_1} \rangle)(\langle x_q^{p_2} \rangle \ldots \langle x_r^{p_2} \rangle) \ldots (\langle x_u^{p_s} \rangle \ldots \langle x_v^{p_s} \rangle)$$

$$= M^{[\rho]} (\mu'_{p_1} \ldots \mu'_{p_1})(\mu'_{p_2} \ldots \mu'_{p_2}) \ldots (\mu'_{p_s} \ldots \mu'_{p_s})$$

$$= M^{[\rho]} \mu'^{\lambda_1}_{p_1} \mu'^{\lambda_2}_{p_2} \ldots \mu'^{\lambda_s}_{p_s} \quad . \tag{B19}$$

It is Theorem (B19) for the expectation value that makes augmented symmetric functions so useful. Returning to the example discussed at the beginning of the section, we can write m_2 in terms of augmented symmetric functions by substituting Eqs. (B14a) and (B14b) in Eq. (B13), leading to

$$m_2 = \frac{(M-1)}{M^2} [2] - \frac{1}{M^2} [1^2] \quad . \tag{B20}$$

There are easier ways of finding m_2 in terms of augmented symmetric functions than that employed above. Moments can be expressed in terms of <u>power sum statistics</u> which are in turn tabulated in terms of augmented symmetric functions. Examples of power sums are

$$(1) = \Sigma\, x_i \tag{B21a}$$

$$(2) = \Sigma\, x_i^2 \quad . \tag{B21b}$$

The r-th power sum can be defined as

$$(r) = \Sigma\, x_i^r \tag{B22a}$$

or

$$= M m'_r \tag{B22b}$$

as can be seen from Eq. (38). From Eq. (B6), we know that

$$m_2 = \frac{1}{M} \Sigma\, x_i^2 - \frac{1}{M^2} (\Sigma x_i)^2$$

or in terms of the power sums (1) and (2),

$$m_2 = \frac{1}{M} (2) - \frac{1}{M^2} (1)^2 \quad . \tag{B23}$$

We can evaluate $(1)^2$ in terms of augmented symmetric functions by substituting Eqs. (B14a), (B14b), and (B21a) in Eq. (B8):

$$(1)^2 = [2] + [1^2] \; . \tag{B24}$$

By comparing the definitions for augmented symmetric functions and power sums, Eqs. (B15) and (B22), we can see that

$$[r] = (r) \; ; \tag{B25}$$

$$[2] = (2) \; . \tag{B26}$$

We substitute Eqs. (B24) and (B26) into Eq. (B23) and find that

$$\begin{aligned} m_2 &= \frac{1}{M}[2] - \frac{1}{M^2}([2] + [1^2]) \\ &= \frac{(M-1)}{M^2}[2] - \frac{1}{M^2}[1^2] \; . \end{aligned} \tag{B27}$$

Equation (B19) shows us how to find the expectation values of [2] and $[1^2]$,

$$\langle [2] \rangle = M \mu_2' \tag{B28a}$$

$$\langle [1^2] \rangle = M(M-1)\, \mu_1'^2 \; . \tag{B28b}$$

The expectation value of m_2 is then

$$\begin{aligned} \langle m_2 \rangle &= \left\langle \frac{(M-1)}{M^2}[2] - \frac{1}{M^2}[1^2] \right\rangle \\ &= \frac{(M-1)}{M^2}\langle [2] \rangle - \frac{1}{M^2}\langle [1^2] \rangle \\ &= \frac{(M-1)M}{M^2}\mu_2' - \frac{M(M-1)}{M^2}\mu_1'^2 \\ &= \frac{(M-1)}{M}(\mu_2' - \mu_1'^2) \; . \end{aligned}$$

We arrive at the same result for $\langle m_2 \rangle$ as given by Eq. (B11).

Equations (B24) and (B26) were derived only for heuristic purposes. Ordinarily, if we wanted to find a power sum or product of power sums in terms of augmented symmetric functions, or vice versa, we would consult a table such as Table B2 below.

TABLE B2 - Augmented symmetric functions and power sums of weight 2.

	[2]	$[1^2]$
(2)	I	-1
$(1)^2$	1	I

This table implies that

$$(2) = [2]$$

$$(1)^2 = [2] + [1^2]$$

$$[2] = (2)$$

$$[1^2] = -(2) + (1)^2.$$

To express a given augmented symmetric function in terms of power sums, read the corresponding <u>column</u> from top to bottom, down to and including the diagonal element. To express a given product of power sums in terms of augmented symmetric functions, read the corresponding <u>row</u> from left to right, up to and including the diagonal element. Note that in Table B2 and elsewhere, each diagonal element "1" is written as I: "capital" one.

Table B2 is said to be a table of weight 2. The weight of a table is the same as the weight of the augmented symmetric functions in that table. For the augmented symmetric function $[p_1^{\lambda_1} p_2^{\lambda_2} \ldots p_s^{\lambda_s}]$, the weight p is defined as

$$p \equiv p_1\lambda_1 + p_2\lambda_2 + \ldots p_s\lambda_s \,. \tag{B29}$$

The weight of both [2] and $[1^2]$ is 2; clearly then the weight of Table B2 must be 2.

3. Direct Calculation of $\hat{\mu}_2$

So far, we have only confirmed a stated relation, i.e. that $\hat{\mu}_2 = Mm_2/(M-1)$. We still require a routine procedure for arriving at the unbiased estimator of an arbitrary moment. For this, μ_2 must be reduced to a sum of population values that have easily derived unbiased estimators. The most obvious class of population values possessing this property are the parent moments about zero. From Eq. (B19) we can deduce that the unbiased estimator of a product of parent moments about zero is

$$U(\mu'^{\lambda_1}_{p_1} \mu'^{\lambda_2}_{p_2} \ldots \mu'^{\lambda_s}_{p_s}) = [p_1^{\lambda_1} p_2^{\lambda_2} \ldots p_s^{\lambda_s}]/M^{[\rho]} \,, \tag{B30}$$

where $\rho = \lambda_1 + \lambda_2 + \ldots \lambda_s$.

From Eq. (B12), we know that μ_2 can be expressed in terms of parent moments about zero as

$$\mu_2 = \mu'_2 - (\mu'_1)^2 \,.$$

Because the unbiased estimator of a sum is equal to the sum of the unbiased estimators for each term, we know that

$$\hat{\mu}_2 = U(\mu_2') - U(\mu_1'^2) \quad .$$

Equation (B30) allows us to conclude that

$$\hat{\mu}_2 = \frac{[2]}{M^{[1]}} - \frac{[1^2]}{M^{[2]}}$$

$$= \frac{[2]}{M} - \frac{[1^2]}{M(M-1)} \quad . \qquad \text{(B31)}$$

Table B2 implies that

$$[2] = (2)$$

$$[1^2] = -(2) + (1)^2,$$

so that

$$\hat{\mu}_2 = \frac{(2)}{M} - \left\{ \frac{-(2) + (1)^2}{M(M-1)} \right\}$$

$$= \frac{(2)}{M} + \frac{(2)}{M(M-1)} - \frac{(1)^2}{M(M-1)}$$

$$= \frac{(2)}{(M-1)} - \frac{(1)^2}{M(M-1)}$$

$$= \left(\frac{M}{M-1}\right) \left\{ \frac{(2)}{M} - \frac{(1)^2}{M^2} \right\} \quad . \qquad \text{(B32)}$$

We recall from Eq. (B22) that

$$(r) = M m_r' \quad .$$

Equation (B32) can then be written in the equivalent form

$$\hat{\mu}_2 = \left(\frac{M}{M-1}\right) \{m_2' - (m_1')^2\} \quad .$$

Equation (B23) implies that $m_2 = m_2' - (m_1')^2$; therefore

$$\hat{\mu}_2 = \frac{M}{M-1} m_2 \ .$$

There are other ways of achieving this result. First, however, we must introduce additional functions - cumulants and k-statistics - which reduce the derivation of unbiased estimators to a routine.

4. Cumulants

We have seen that the parent moments about zero are both simply defined and easy to use for finding expectation values and unbiased estimators. There is a major drawback however, in their application; the value of any moment about zero is dependent on the choice of the origin. Because many calculations involve quantities that are independent of the choice of origin, there is a need for an origin-independent population value.

We can gain some insight into this problem by examining the r-th parent moment about zero μ_r' for a continuous probability density function f(x),

$$\mu_r' = \int_{-\infty}^{\infty} x^r \ f(x)dx \ . \tag{B33}$$

Also corresponding to f(x) is the characteristic function $\phi(t)$ which is defined as

$$\phi(t) \equiv \int_{-\infty}^{\infty} e^{itx} \ f(x)dx \ . \tag{B34}$$

The argument of the exponential is complex, so that the integral can be defined for a wide variety of functions. We can expand the exponential in Eq. (B34) and obtain a different though equivalent form for $\phi(t)$,

$$\phi(t) = \int_{-\infty}^{\infty}(1 + \frac{(itx)}{1!} + \frac{(itx)^2}{2!} + \ldots)\ f(x)dx,$$

$$= (\int_{-\infty}^{\infty} f(x)dx) + (\int_{-\infty}^{\infty} x\ f(x)dx)\cdot\frac{(it)}{1!}$$

$$+ (\int_{-\infty}^{\infty} x^2 f(x)dx)\ \frac{(it)^2}{2!} + \ldots \quad ; \tag{B35}$$

by substituting Eq. (B33) into Eq. (B35), we find that

$$\phi(t) = 1 + \mu_1' \frac{(it)}{1!} + \mu_2' \frac{(it)^2}{2!} + \ldots \quad . \tag{B36}$$

We can use the characteristic function to generate μ_r' by employing the simple algorithm

$$\mu_r' = (-i \frac{d}{dt})^r\ \phi(t)\Big|_{t=0} \quad . \tag{B37}$$

We have previously remarked that one of the disadvantages of working with moments about zero is that the value of such moments depends on the choice of origin. If, for instance, we were to augment the value of the origin by c, the corresponding moment $\mu_r'(c)$ would be

$$\mu_r'(c) = (-i \frac{d}{dt})^r \int_{-\infty}^{\infty} e^{it(x-c)} f(x)dx\Big|_{t=0}$$

$$= (-i \frac{d}{dt})^r\ e^{-itc} \int_{-\infty}^{\infty} e^{itx}\ f(x)dx\Big|_{t=0}$$

$$= (-i \frac{d}{dt})^r\ e^{-itc}\ \phi(t)\Big|_{t=0} \quad . \tag{B38}$$

In general, $\mu_r'(c)$ promises to be very different from μ_r'. Suppose however, that we define a new population value κ_r by the cumulant generating

function log $\phi(t)$ so that

$$\kappa_r \equiv \left(-i \frac{d}{dt}\right)^r \log \phi(t)\Big|_{t=0} . \tag{B39}$$

If we were to change the origin by c again, but this time generate $\kappa_r(c)$, we would find that

$$\kappa_r(c) = \left(-i \frac{d}{dt}\right)^r \log\left(\int_{-\infty}^{\infty} e^{it(x-c)} dx\right)\Big|_{t=0}$$

$$= \left(-i \frac{d}{dt}\right)^r \log\left(e^{-itc} \int_{-\infty}^{\infty} e^{itx} dx\right)\Big|_{t=0}$$

$$= \left(-i \frac{d}{dt}\right)^r (-itc + \log \phi(t))\Big|_{t=0}$$

$$= \left[\left(-i \frac{d}{dt}\right)^r -itc + \kappa_r\right]\Big|_{t=0}$$

$$= -c\, \delta_{1r} + \kappa_r$$

or $$= \kappa_r \text{ for } r > 1 , \tag{B40}$$

where δ_{1r} is Kronecker's delta. These population values, called cumulants, are invariant with respect to the choice of origin except for the first, which is decreased by c.

Cumulants can also be related to the cumulant generating function by

$$\log \phi(t) = \frac{(it)}{1!} \kappa_1 + \frac{(it)^2}{2!} \kappa_2 + \ldots \frac{(it)^r}{r!} \kappa_r + \ldots , \tag{B41}$$

this is simply a solution to Eq. (B39). We can substitute Eq. (B36) into Eq. (B41) and see that cumulants are related to moments about zero through

$$\log(1 + \frac{\mu_1'(it)}{1!} + \ldots \frac{\mu_r'(it)^r}{r!} + \ldots)$$

$$= \varkappa_1 \frac{(it)}{1!} + \varkappa_2 \frac{(it)^2}{2!} + \ldots + \varkappa_r \frac{(it)^r}{r!} + \ldots \tag{B42}$$

or equivalently

$$\log(1 + \frac{\mu_1' t}{1!} + \ldots \frac{\mu_r' t^r}{r!} + \ldots)$$

$$= \frac{\varkappa_1 t}{1!} + \frac{\varkappa_2 t^2}{2!} + \ldots + \frac{\varkappa_r t^r}{r!} + \ldots \tag{B43}$$

and

$$1 + \frac{\mu_1' t}{1!} + \ldots \frac{\mu_r' t^r}{r!} + \ldots$$

$$= \exp\{\frac{\varkappa_1 t}{1!} + \frac{\varkappa_2 t^2}{2!} + \ldots \frac{\varkappa_r t^2}{r!} + \ldots\} . \tag{B44}$$

An explicit expression for the r-th cumulant $\varkappa_r$ in terms of moments about zero can be found by expanding the logarithm in Eq. (B43) and picking out powers of t^r. That is,

$$\varkappa_r = r! \sum \frac{(-1)^{\rho-1}(\rho-1)!}{\lambda_1! \, \lambda_2! \ldots} \left(\frac{\mu'_{p_1}}{p_1!}\right)^{\lambda_1} \left(\frac{\mu'_{p_2}}{p_2!}\right)^{\lambda_2} \ldots \tag{B45}$$

where the sum is over the partition of the integer r such that $p_1\lambda_1 + p_2\lambda_2 + \ldots = r$ and $\lambda_1 + \lambda_2 + \ldots = \rho$. Similarly, an explicit expression for the r-th parent moment about zero in terms of cumulants can be found by expanding Eq. (B44),

$$1 + \frac{\mu_1' t}{1!} + \ldots \frac{\mu_r' t^r}{r!} + \ldots$$

$$= \exp(\frac{\varkappa_1 t}{1!}) \exp(\frac{\varkappa_2 t}{2!}) \ldots \exp(\frac{\varkappa_r t^r}{r!}) \ldots$$

$$= \{1 + \frac{\varkappa_1 t}{1!} + \frac{\varkappa_1^2 t^2}{2!} + \ldots\}\{1 + \frac{\varkappa_2 t^2}{2!} + \frac{1}{2}\left(\frac{\varkappa_2 t^2}{2!}\right)^2 + \ldots\} \ldots$$

$$\times \{1 + \frac{\varkappa_r t^r}{r!} + \frac{1}{2!}\left(\frac{\varkappa_r t^r}{r!}\right)^2 + \ldots\} \ldots \tag{B46}$$

and then picking out the terms in the exponential expansion which, when multiplied together, give a power t^r. We therefore have

$$\mu'_r = \sum \frac{r!}{\lambda_1!\,\lambda_2!\,\ldots}\left(\frac{\kappa_{p_1}}{p_1!}\right)^{\lambda_1}\left(\frac{\kappa_{p_2}}{p_2!}\right)^{\lambda_2}\ldots \tag{B47}$$

where the sum is over the partition of the integer r such that $p_1\lambda_1 + p_2\lambda_2 + \ldots = r$.

By choosing the origin of the distribution so that $\mu'_1 = 0$, the cumulants can be written in terms of moments about the mean. For example

$$\begin{aligned}\kappa_4 &= \mu'_4 - 4\mu'_3\mu'_1 - 3\mu'^2_2 + 12\mu'_2\mu'^2_1 - 6\mu'^4_1\\ &= \mu_4 - 3\mu_2^2 \;.\end{aligned}$$

Equation (B47) can be used to show that $\kappa_1 = \mu'_1$. If we assume that $\mu'_1 = 0$, the expressions for parent moments about the mean, in terms of cumulants, are often considerably simpler than the corresponding expressions for parent moments about zero. For example, for the fourth moment about zero, we have

$$\mu'_4 = \kappa_4 + 4\kappa_3\kappa_1 + 3\kappa_2^2 + 6\kappa_2\kappa_1^2 + \kappa_1^4 ;$$

for the moment about mean, however,

$$\mu_4 = \kappa_4 + 3\kappa_2^2 \;.$$

Therefore from Eq. (B47), we can write the second through eighth parent moments about the mean in terms of cumulants as

$$\mu_2 = \kappa_2 \tag{B48a}$$

$$\mu_3 = \kappa_3 \tag{B48b}$$

$$\mu_4 = \kappa_4 + 3\kappa_2^2 \tag{B48c}$$

$$\mu_5 = \kappa_5 + 10\kappa_3\kappa_2 \tag{B48d}$$

$$\mu_6 = \kappa_6 + 15\kappa_4\kappa_2 + 10\kappa_3^2 + 15\kappa_2^3 \tag{B48e}$$

$$\mu_7 = \kappa_7 + 21\kappa_5\kappa_2 + 35\kappa_4\kappa_3 + 105\kappa_3\kappa_2^2 \tag{B48f}$$

$$\mu_8 = \kappa_8 + 28\kappa_6\kappa_2 + 56\kappa_5\kappa_3 + 35\kappa_4^2 + 210\kappa_4\kappa_2^2$$
$$+ 280\kappa_3^2\kappa_2 + 105\kappa_2^4 \quad . \tag{48g}$$

Similarly, Eq. (B45) can be used to show that

$$\kappa_2 = \mu_2 \tag{B49a}$$

$$\kappa_3 = \mu_3 \tag{B49b}$$

$$\kappa_4 = \mu_4 - 3\mu_2^2 \tag{B49c}$$

$$\kappa_5 = \mu_5 - 10\mu_3\mu_2 \tag{B49d}$$

$$\kappa_6 = \mu_6 - 15\mu_4\mu_2 - 10\mu_3^2 + 30\mu_2^3 \tag{B49e}$$

$$\kappa_7 = \mu_7 - 21\mu_5\mu_2 - 35\mu_4\mu_3 + 210\mu_3\mu_2^2 \tag{B49f}$$

$$\kappa_8 = \mu_8 - 28\mu_6\mu_2 - 56\mu_5\mu_3 - 35\mu_4^2 + 420\mu_4\mu_2^2$$
$$+ 560\mu_3^2\mu_2 - 630\mu_2^4 \quad . \tag{B49g}$$

5. k-statistics

So far, we have only shown how moments are related to cumulants. We have not yet shown how cumulants can be used to find the unbiased estimators of parent moments. Because every parent moment can be expressed

as a sum of cumulant products, a way of finding the unbiased estimator of a cumulant product could facilitate the search for an unbiased estimator of a parent moment. Equation (B45) gives us an expression for a single cumulant. The equivalent expression for a product of cumulants $\kappa_r\kappa_s\kappa_t\ldots$ is

$$\kappa_r\kappa_s\ldots = r!s!\ldots\prod\left[\sum\frac{(-1)^{\rho-1}(\rho-1)!}{\lambda_1!\,\lambda_2!\,\ldots}\left(\frac{\mu'_{p_1}}{p_1!}\right)^{\lambda_1}\left(\frac{\mu'_{p_2}}{p_2!}\right)^{\lambda_2}\ldots\right]; \qquad \text{(B50)}$$

the symbol π indicates that we are taking the product of the sums corresponding to the cumulants that comprise the cumulant product $\kappa_r\kappa_s\ldots$. In Section 10, we find that this product can also be expressed as

$$\kappa_r\kappa_s\ldots = r!s!\ldots\sum\frac{(-1)^{\Sigma(\rho-1)}\pi\{(\rho-1)!\}}{\pi\{(\lambda_1!\lambda_2!\ldots)\}}\prod\left[\left(\frac{\mu'_{p_1}}{p_1!}\right)^{\lambda_1}\left(\frac{\mu'_{p_2}}{p_2!}\right)^{\lambda_2}\ldots\right] \qquad \text{(B51)}$$

where for the index of the *first cumulant* product, namely r, we have a partition of the integer r such that $p_1\lambda_1 + p_2\lambda_2 + \ldots = r$ and $\lambda_1 + \lambda_2 + \ldots = \rho$. There are similar partitions of the indices s,t ..., and inside the large summation the symbols π and Σ are used to denote multiplications and sums to cover all of r, s, t ..., while the large summation sign denotes that we must sum over all partitions [11].

Now that we know how to represent a cumulant product as a sum of moment products, we can use Eq. (B30) to find the unbiased estimator of $\kappa_r\kappa_s\ldots$:

$$U(\kappa_r\kappa_s \ldots) = r!s! \ldots \sum \frac{(-1)^{\Sigma(\rho-1)}\pi\{(\rho-1)!\}}{\pi\{(\lambda_1!\ \lambda_2!\ \ldots)\}} U\left(\pi\left[\left(\frac{\mu'_{p_1}}{p_1!}\right)^{\lambda_1}\left(\frac{\mu'_{p_2}}{p_2!}\right)^{\lambda_2}\ldots\right]\right)$$

$$= r!s! \ldots \sum \frac{(-1)^{\Sigma(\rho-1)}\pi\{(\rho-1)!\}}{\pi\{(\lambda_1!\ \lambda_2!\ \ldots)\}} \frac{U\{\pi(\mu'^{\lambda_1}_{p_1}\ \mu'^{\lambda_2}_{p_2}\ldots)\}}{\pi\{(p_1!)^{\lambda_1}(p_2!)^{\lambda_2}\ldots\}}$$

$$= r!s! \ldots \sum \frac{(-1)^{\Sigma(\rho-1)}\ \pi\{(\rho-1)!\}}{\pi\{(\lambda_1!\ \lambda_2!\ \ldots)\}} \frac{[\pi(p_1^{\lambda_1}\ p_2^{\lambda_2}\ldots)]/M^{[\rho]}}{\pi\{(p_1!)^{\lambda_1}(p_2!)^{\lambda_2}\ \ldots\}}\ . \qquad (B52)$$

We call the unbiased estimator of $\kappa_r\kappa_s$ ... the k-statistic k_{rs}... . That is

$$k_{rs} \equiv U(\kappa_r\kappa_s \ldots) \qquad (B53a)$$

or

$$= \sum \frac{(-1)^{\Sigma(\rho-1)}\ \pi\{(\rho-1)!\}}{\pi\{\lambda_1!\ \lambda_2!\ \ldots\}} \frac{r!s!\ldots}{\pi\{(p_1!)^{\lambda_1}(p_2!)^{\lambda_2}\ldots\}} \frac{[\pi(p_1^{\lambda_1}p_2^{\lambda_2}\ldots)]}{M^{[\Sigma\rho]}}\ , \qquad (B53b)$$

where the sums and products are taken over the same partitions and indices as in Eq. (B51).

To illustrate, let us work out k_{32}. The partitions of 3 are 3, 21 and 1^3, and of 2 they are 2 and 1^2. We shall therefore have terms in [32], [31^2], [2^21], [21^3], and [1^5]. The first term is

$$\frac{(-1)^{0+0}0!.0!}{1!.1!}\ \frac{3!.2!}{(3!)^1(2!)^1}\ \frac{[3.2]}{M^{[1+1]}} = \frac{[32]}{M^{[2]}}$$

This is followed by

$$\frac{(-1)^{0+1}0!.1!}{1!\ 2!}\ \frac{3!2!}{(3!).(1!)^2}\ \frac{[3.1^2]}{M^{[1+2]}} = -\frac{[31^2]}{M^{[3]}} ,$$

and by

$$\frac{(-1)^{1+0}1!.0!}{1!1!.1!}\ \frac{3!.2!}{(2!)^1(1!)^1.(2!)^1}\ \frac{[21.2]}{M^{[2+1]}} = -\frac{3[2^21]}{M^{[3]}} .$$

The fourth term, however, consists of two parts, namely

$$\frac{(-1)^{2+0}2!.0!}{3!.1!}\ \frac{3!.2!}{(1!)^3.2!}\ \frac{[1^3.2]}{M^{[3+1]}} = \frac{2[21^3]}{M^{[4]}}$$

and

$$\frac{(-1)^{1+1}1!.1!}{1!1!.2!}\ \frac{3!.2!}{2!1!.(1!)^2}\ \frac{[21.1^2]}{M^{[2+2]}} = \frac{3[21^3]}{M^{[4]}}$$

$$= \frac{5[21^3]}{M^{[4]}}$$

while the last term is

$$\frac{(-1)^{2+1}2!.1!}{3!2!}\ \frac{3!.2!}{(1!)^3.(1!)^2}\ \frac{[1^3.1^2]}{M^{[3+2]}} = -\frac{2[1^5]}{M^{[5]}} .$$

Therefore, we have that [11]

$$k_{32} = \frac{[32]}{M^{[2]}} - \frac{[31^2]}{M^{[3]}} - \frac{3[2^21]}{M^{[3]}} + \frac{5[21^3]}{M^{[4]}} - \frac{2[1^5]}{M^{[5]}} .$$

Fortunately, many k-statistics have been tabulated in terms of augmented symmetric functions. These tables are arranged according to the order of the k-statistics and the augmented symmetric functions in the table. The order of a k-statistic is equal to the sum of its indices; the order of an augmented symmetric function equals its weight as defined by Eq. (B29). For example k_{111} is of order 3 and k_{321} is of order six.

The first order table is

$$k_1 = [1]/M \; . \tag{B54}$$

The second order table of k-statistics and augmented symmetric functions are shown in Table B3.

TABLE B3 - k-statistics and augmented symmetric functions of weight 2.

	k_{11}	k_2
$[1^2]/M^{[2]}$	1	-1
$[2]/M$	1	1

The conventions for reading Table B3 are the same as reading Table B2. Thus

$$[1^2]/M^{[2]} = k_{11}$$

$$[2]/M = k_{11} + k_2$$

$$k_{11} = [1^2]/M^{[2]}$$

$$k_2 = -[1^2]/M^{[2]} + [2]/M \; .$$

We have now acquired most of the tools needed to find the unbiased estimator of a moment. Next, we will state an algorithm for using these tools and apply the algorithm to two examples.

6. Algorithm B1: Finding the Unbiased Estimator of a Population Value

At this point, we choose to outline the preferred method for calculating the unbiased estimator of a population value.

a. Find the population value in terms of cumulant products. If the population value is in terms of parent moments, this can be done by employing Eqs. (B48a)-(B48g).

b. Convert each cumulant product to its corresponding k-statistic, in accord with Eq. (B53a).

c. Using the k-statistic/augmented symmetric function table of the same order as the k-statistic, find each k-statistic as a sum of augmented symmetric functions.

d. Using the augmented symmetric function/power sum table of order r, find each augmented symmetric function as a sum of power sum products.

e. Replace each power sum (r) by a power sum about the mean s_r, defined as

$$s_r = \sum_{i=1}^{M} (x_i - m_1')^r = Mm_r \ . \tag{B55}$$

This substitution is justified by the fact that the value of any k-statistic is independent of the choice of the origin, so the convenient choice is one such that $m_1' = 0$ and therefore $s_1 = 0$. The resulting unbiased estimator can then be expressed in terms of sample moments about the mean.

7. Algorithm B1 as Applied to μ_2

a. Find μ_2 in terms of cumulants by Eq. (B48a), $\mu_2 = \kappa_2$.

b. Find the k-statistic corresponding to κ_2. According to Eq. (B53a), $\hat{\kappa}_2 = k_2$ and therefore $\hat{\mu}_2 = k_2$.

c. Find k_2 in terms of augmented symmetric functions via a 2nd order table such as Table B3. We thus find

$$k_2 = -[1^2]/M^{[2]} + [2]/M.$$

Therefore

$$\hat{\mu}_2 = k_2 = [2]/M - [1^2]/(M(M-1)) .$$

d. Find the augmented symmetric functions in terms of power sums. From Table B2, we know that

$$[2] = (2)$$

$$[1^2] = -(2) + (1)^2 .$$

The unbiased estimator $\hat{\mu}_2$ can thus be expressed in terms of power sums as

$$\begin{aligned}\hat{\mu}_2 &= \frac{1}{M}\left([2] - [1^2]/(M-1)\right)\\ &= \frac{1}{M}\left[(2) - ((1)^2 - (2))/(M-1)\right]\\ &= \frac{1}{M}\{(2)[1 + 1/(M-1)] - (1)^2/(M-1)\} .\end{aligned}$$

e. Replace each power sum by a power sum about the mean as defined by Eq. (B55),

$$\mu_2 = \frac{1}{M}\{s_2(\frac{M}{M-1}) - s_1^2/(M-1)\} .$$

However because $s_1 = 0$, this simplifies to

$$\mu_2 = \frac{1}{M}\{s_2 \frac{M}{M-1}\} .$$

f. Express the unbiased estimator $\hat{\mu}_2$ in terms of sample moments about the mean. That is

$$\hat{\mu}_2 = \frac{M}{M-1} \frac{s_2}{M} = \frac{M}{M-1} m_2 .$$

8. Algorithm B1 as Applied to μ_4.

a. Equation (B48c) enables us to find μ_4 in terms of cumulants as

$$\mu_4 = \kappa_4 + 3\kappa_2^2 .$$

b. Because of Eq. (B53a), we can express $\hat{\mu}_4$ in terms of k-statistics as

$$\hat{\mu}_4 = k_4 + 3k_{22} .$$

c. These two k-statistics are both of fourth order; we can find each of them in terms of augmented symmetric functions via a fourth order table such as Table B4 below.

TABLE B4 - k-statistics and augmented symmetric functions of weight 4.

	k_{1111}	k_{211}	k_{22}	k_{31}	k_4
$[1^4]/M^{[4]}$	I	-1	1	2	-6
$[21^2]/M^{[3]}$	1	I	-2	-3	12
$[2^2]/M^{[2]}$	1	2	I		-3
$[31]/M^{[2]}$	1	3		I	-4
$[4]/M$	1	6	3	4	I

From B4 we find that

$$k_4 = -6[1^4]/M^{[4]} + 12[21^2]/M^{[3]} - 3[2^2]/M^{[2]} - 4[31]/M^{[2]}$$
$$+ [4]/M$$

$$k_{22} = [1^4]/M^{[4]} - 2[21^2]/M^{[3]} + [2^2]/M^{[2]} .$$

Therefore, $\hat{\mu}_4$ can be expressed in terms of augmented symmetric functions as

$$\hat{\mu}_4 = -\frac{6[1^4]}{M^{[4]}} + \frac{12[21^2]}{M^{[3]}} - \frac{3[2^2]}{M^{[2]}} - \frac{4[31]}{M^{[2]}} + \frac{[4]}{M}$$

$$+ 3\{\frac{[1^4]}{M^{[4]}} - \frac{2[21^2]}{M^{[3]}} + \frac{[2^2]}{M^{[2]}}\} .$$

$$= -\frac{3[1^4]}{M^{[4]}} + \frac{6[21^2]}{M^{[3]}} - \frac{4[31]}{M^{[2]}} + \frac{[4]}{M} .$$

d. Table B5 gives the relation between augmented symmetric functions and power sums of weight 4.

TABLE B5 - Augmented symmetric functions and power sums of weight 4.

	[4]	[31]	$[2^2]$	$[21^2]$	$[1^4]$
(4)	I	-1	-1	2	-6
(3)(1)	1	I		-2	8
$(2)^2$	1		I	-1	3
$(2)(1)^2$	1	2	1	I	-6
$(1)^4$	1	4	3	6	I

In Section 2 of this appendix, we learned how to use a table of this kind for finding augmented symmetric functions in terms of power sum products. We therefore know that Table B5 implies that

$$[1^4] = -6(4) + 8(3)(1) + 3(2)^2 - 6(2)(1)^2 + (1)^4$$

$$[21^2] = 2(4) - 2(3)(1) - (2)^2 + (2)(1)^2$$

$$[31] = -(4) + (3)(1)$$

$$[4] = (4) \quad .$$

We can now find $\hat{\mu}_4$, in terms of power sum products, as

$$\hat{\mu}_4 = -3[-6(4) + 8(3)(1) + 3(2)^2 - 6(2)(1)^2 + (1)^4]/M^{[4]}$$

$$+ 6[2(4) - 2(3)(1) - (2)^2 + (2)(1)^2]/M^{[3]}$$

$$- 4[-(4) + (3)(1)]/M^{[2]} + (4)/M$$

$$= (4)\left[\frac{1}{M} + \frac{4}{M^{[2]}} + \frac{12}{M^{[3]}} + \frac{18}{M^{[4]}}\right] + (3)(1)\left[\frac{-4}{M^{[2]}} - \frac{12}{M^{[3]}} - \frac{24}{M^{[4]}}\right]$$

$$+ (2)^2\left[-\frac{6}{M^{[3]}} - \frac{9}{M^{[4]}}\right] + (2)(1)^2\left[\frac{6}{M^{[3]}} + \frac{18}{M^{[4]}}\right] - \frac{3(1)^4}{M^{[4]}}$$

$$= (4)\left[\frac{1}{M} + \frac{4}{M^{[2]}} + \frac{12}{M^{[3]}} + \frac{18}{M^{[4]}}\right] - 4(3)(1)\left[\frac{1}{M^{[2]}} + \frac{3}{M^{[3]}} + \frac{6}{M^{[4]}}\right]$$

$$- 3(2)^2\left[\frac{2}{M^{[3]}} + \frac{3}{M^{[4]}}\right] + 6(2)(1)^2\left[\frac{1}{M^{[3]}} + \frac{3}{M^{[4]}}\right] - \frac{3(1)^4}{M^{[4]}}$$

e. The expression for $\hat{\mu}_4$ can be greatly simplified by substituting power sums about the mean for the power sums; without loss of generality we can assume that $s_1 = 0$ and obtain the simplified expression

$$\hat{\mu}_4 = s_4\left[\frac{1}{M} + \frac{4}{M^{[2]}} + \frac{12}{M^{[3]}} + \frac{18}{M^{[4]}}\right] - 3s_2^2\left[\frac{2}{M^{[3]}} + \frac{3}{M^{[4]}}\right] .$$

f. In terms of sample moments about the mean, $\hat{\mu}_4$ now appear

$$\hat{\mu}_4 = m_4\left[1 + \frac{4}{(M-1)} + \frac{12}{(M-1)^{[2]}} + \frac{18}{(M-1)^{[3]}}\right] - 3m_2^2\left[\frac{2M}{(M-1)^{[2]}} + \frac{3M}{(M-1)^{[3]}}\right] .$$

9. Algorithm B2: Another Method for Evaluating k-statistics [12]

We have already shown how to find a k-statistic of order m in terms of augmented symmetric functions from a table of order m. The purpose of this section is to show how to evaluate a k-statistic of order m, given a table of a larger order n. This method is outlined below.

a. We want to find the m-th order k-statistic $k_{rs}\ldots$ from on n-th order table. This is accomplished by first finding the n-th order k-statistic $k_{rs\ldots 1^{(n-m)}}$ in terms of augmented symmetric functions. For instance, if we wanted to find k_2 from a fourth order table, we would first have to find k_{211} or equivalently k_{21^2}.

b. Notice that the k-statistic $k_{rs\ldots 1^{(n-m)}}$ can be represented as a sum of symmetric functions which all contain unity to at least the (n-m)th power. For example, Table B4 implies that k_{211} can be represented in terms of augmented symmetric functions as

$$k_{211} = -[1^4]/M^{[4]} + [21^2]/M^{[3]}.$$

In this case, (n-m) is equal to 2; we can see that each augmented symmetric function contains unity to the second power. It is also true that the argument u for all $M^{[u]}$'s in the expansion for $k_{rs\ldots 1^{(n-m)}}$ is as least

as large as (n-m). For the case of k_{211}, arguments of $M^{[4]}$ and $M^{[3]}$ are both obviously greater than two.

c. In order to find $k_{rs\ldots}$ from $k_{rs\ldots 1^{(n-m)}}$, we simply reduce all powers of one in the associated augmented symmetric functions and all arguments of $M^{[u]}$ by (n-m). From k_{21^2}, we could then find that k_2 is

$$k_{21^{(2-2)}} = k_2$$

$$= -[1^{4-2}]/M^{[4-2]} + [21^{(2-2)}]/M^{[3-2]}$$

$$= -[1^2]/M^{[2]} + [2]/M \ ,$$

as can be verified from Table B3.

We can prove this algorithm by considering Eq. (B53a), the definition of the k-statistic $k_{rs\ldots}$,

$$k_{rs\ldots} = U(\varkappa_r \varkappa_s \ldots). \tag{B56}$$

It follows that

$$k_{rs\ldots 1^{(n-m)}} = U(\varkappa_r \varkappa_s \ldots \varkappa_1^{(n-m)}) \ . \tag{B57}$$

Because $\varkappa_1 = \mu_1'$, we also know that

$$k_{rs\ldots 1^{(n-m)}} = U(\varkappa_r \varkappa_s \ldots \mu_1'^{(n-m)}) \ . \tag{B58}$$

From Eq. (B51), however,

$$\varkappa_r \varkappa_s \ldots \mu_1'^{(n-m)} =$$

$$r!s!\ldots \sum \frac{(-1)^{\Sigma(\rho-1)} \ \pi\{(\rho-1)!\}}{\pi\ \{(\lambda_1!\lambda_2!\ \ldots)\}} \prod \left\{ \left(\frac{\mu'_{p_1}}{p_1!}\right)^{\lambda_1} \left(\frac{\mu'_{p_2}}{p_2!}\right)^{\lambda_2} \ldots \right\} \mu_1'^{(n-m)} \ . \tag{B59}$$

We can use Eq. (B30) to find $k_{rs\ldots 1}(n-m)$ from Eq. (B53b). That is,

$$k_{rs\ldots 1}(n-m) =$$

$$\sum \frac{(-1)^{\Sigma(\rho-1)}\,\pi\{(\rho-1)!\}}{\pi\{\lambda_1!\lambda_2!\ldots\}} \; \frac{r!s!}{\pi\{(p_1!)^{\lambda_1}(p_2!)^{\lambda_2}\ldots\}} \; \frac{[\pi(p_1^{\lambda_1}p_2^{\lambda_2}\ldots 1^{(n-m)})]}{M^{[\Sigma\rho+(n-m)]}} . \tag{B60}$$

However, we know from Eq. (B53b) that $k_{rs\ldots}$ can be represented as

$$k_{rs\ldots} =$$

$$\sum \frac{(-1)^{\Sigma(\rho-1)}\,\pi\{(\rho-1)!\}}{\pi\{\lambda_1!\lambda_2!\ldots\}} \; \frac{r!s!}{\pi\{(p_1!)^{\lambda_1}(p_2!)^{\lambda_2}\ldots\}} \; \frac{[\pi(p_1^{\lambda_1}p_2^{\lambda_2}\ldots)\}]}{M^{[\Sigma\rho]}} .$$

Notice that the coefficient corresponding to each term $[\pi(p_1^{\lambda_1}p_2^{\lambda_2}\ldots)]/M^{[\Sigma\rho]}$ in $k_{rs\ldots}$ is identical to the coefficient corresponding to each term $[\pi(p_1^{\lambda_1}p_2^{\lambda_2}\ldots)1^{(n-m)}]/M^{[\Sigma\rho+(n-m)]}$ in $k_{rs\ldots 1}(n-m)$. For example, the coefficient corresponding to each term $[2]/M^{[1]}$ in k_2 is identical to the coefficient corresponding to each term $[21^2]/M^{[3]}$ in k_{211}. This, of course, is the same principle used in the algorithm outlined above.

10. Partitions as Employed in Defining Cumulants and k-statistics

We have already noted in Eq. (B45), that

$$\kappa_r = r!\sum \frac{(-1)^{\rho-1}(\rho-1)!}{\lambda_1!\lambda_2!\ldots}\left(\frac{\mu'_{p_1}}{p_1!}\right)^{\lambda_1}\left(\frac{\mu'_{p_2}}{p_2!}\right)^{\lambda_2}\ldots ,$$

where the sum is over the partition of the integer r such that $p_1\lambda_1 + p_2\lambda_2 + \ldots = r$ and $\lambda_1 + \lambda_2 + \ldots = \rho$. An example will clarify the

term partition. Consider the integer 4; the set of combinations belonging to the partition of 4 according to the above prescription is

$$\{4,\ 3+1,\ 2+2,\ 2+1+1,\ 1+1+1+1\} .$$

This partition can be represented more elegantly as

$$\{4,\ 3+1,\ 2\times 2,\ 2+1\times 2,\ 1\times 4\} ,$$

or better yet as

$$\{4^1,\ 3^1 1^1,\ 2^2,\ 2^1 1^2,\ 1^4\} .$$

Every positive integer has a corresponding partition. One possible combination belonging to the partition of r is

$$p_1^{\lambda_1}\ p_2^{\lambda_2}\ \cdots\ p_t^{\lambda_t} ,$$

where, of course,

$$p_1\lambda_1 + p_2\lambda_2 + \dots\ p_t\lambda_t = r .$$

We could be more specific and consider the j-th combination of the partition of r:

$$p_{1j}^{\lambda_{1j}}\ p_{2j}^{\lambda_{2j}}\ \cdots\ p_{tj}^{\lambda_{tj}}$$

or

$$\prod_i p_{ij}^{\lambda_{ij}} .$$

The quantities p_{ij} and λ_{ij} respectively will be called the i-th base and the i-th power of the j-th combination of the partition of r. To each j-th combination there corresponds a sum of its powers ρ_j:

$$\rho_j = \lambda_{1j} + \lambda_{2j} + \dots\ \lambda_{tj}$$

or

$$= \sum_i \lambda_{ij} \quad .$$

Using our new definitions, $\varkappa_r$ can be represented as

$$\varkappa_r = \sum_j \frac{r!(-1)^{\rho_j - 1}(\rho_j - 1)!}{\pi_i\{(p_{ij})!^{\lambda_{ij}}(\lambda_{ij})!\}} \pi_i (\mu'_{p_{ij}})^{\lambda_{ij}} \quad . \tag{B61}$$

or equivalently as

$$\varkappa_r = \sum_j C_j \pi_i (\mu'_{p_{ij}})^{\lambda_{ij}} \quad , \tag{B62a}$$

where

$$C_j = \frac{r!(-1)^{\rho_j - 1}(\rho_j - 1)!}{\pi_i\{(p_{ij})!^{\lambda_{ij}}(\lambda_{ij})!\}} \quad . \tag{B62b}$$

As an example, we compute $\varkappa_3$ using Eq. (B61), by first noticing that the partition of 3 is

$$\{3,\ 2+1,\ 1+1+1\}$$

or

$$\{3^1,\ 2^1 1^1,\ 1^3\} \quad .$$

The first term of $\varkappa_3$ is then

$$C_1 \pi_i (\mu'_{p_{i1}})^{\lambda_{i1}} = \frac{3!(-1)^{\rho_1 - 1}(\rho_1 - 1)!}{\pi_i\{(p_{i1})!^{\lambda_{i1}}(\lambda_{i1})!\}} \pi_i (\mu'_{p_{i1}})^{\lambda_{i1}}$$

$$= \frac{3!(-1)^{1-1}(1-1)!}{(3!)^1(1!)} (\mu'_3)^1$$

$$= \mu'_3 \quad .$$

This is followed by the expression for the term corresponding to the combination $2^1 1^1$ and $j = 2$:

$$C_2 \prod_i (\mu'_{p_{i2}})^{\lambda_{i2}} = \frac{3!(-1)^{\rho_2 - 1}(\rho_2 - 1)!}{\prod_i \{(p_{i2})!^{\lambda_{i2}}(\lambda_{i2})!\}} \prod_i (\mu'_{i2})^{\lambda_{i2}}$$

$$= \frac{3!(-1)^{2-1}(2-1)!}{\{(2!)^1(1!)\}\{(1!)^1(1!)\}} (\mu'_2)^1(\mu'_1)^1$$

$$= -3\mu'_2\mu'_1 \quad .$$

The third term, which corresponds to 1^3, is

$$C_3 \prod_i (\mu_{p_{i3}})^{\lambda_{i3}} = \frac{3!(-1)^{\rho_3 - 1}(\rho_3 - 1)!}{\prod_i \{(p_{i3})!^{\lambda_{i3}}(\lambda_{i3})!\}} \prod_i (\mu'_{p_{i3}})^{\lambda_{i3}}$$

$$= \frac{3!(-1)^{(3-1)}(3-1)!}{\{(1!)^3(3!)\}} (\mu'_1)^3$$

$$= 2\mu'^3_1 \ .$$

We add these 3 expressions together and find that

$$\varkappa_3 = \mu'_3 - 3\mu'_2\mu'_1 + 2\mu'^3_1 \quad . \tag{B63}$$

In Eq. (B61) we represented a single cumulant in terms of parent moments. When dealing with cumulant products, however, more than one partition is is required. For example, in order to express $\varkappa_3\varkappa_2$ in terms of parent

moments, partitions of 3 and 2 are involved. An index is necessary to show which partition a given λ_{ij}, p_{ij}, or ρ_j belongs to. We let the index m identify the particular partition to which λ_{ijm}, p_{ijm}, and ρ_{ijm} belong. The r_mth cumulant is then

$$\varkappa_{r_m} = \sum_j \frac{r_m!(-1)^{\rho_{jm}-1}(\rho_{jm}-1)!}{\pi_i \{(p_{ijm})!^{\lambda_{ijm}}(\lambda_{ijm})!\}} \pi_i (\mu'_{p_{ijm}})^{\lambda_{ijm}} \tag{B64a}$$

or

$$= \sum_j C_{jm} \pi_i (\mu'_{p_{ijm}})^{\lambda_{ijm}} , \tag{B64b}$$

where

$$C_{jm} = \frac{r_m!(-1)^{\rho_{jm}-1}(\rho_{jm}-1)!}{\pi_i \{(p_{ijm})!^{\lambda_{ijm}}(\lambda_{ijm})!\}} . \tag{B65}$$

A product of cumulants is

$$\varkappa_{r_1}\varkappa_{r_2}\dots = \pi_m \varkappa_{rm}$$

$$= \prod_m \left(\sum_j \frac{r_m!(-1)^{\rho_{jm}-1}(\rho_{jm}-1)!}{\pi_i \{(p_{ijm})!^{\lambda_{ijm}}(\lambda_{ijm})!\}} \pi_i (\mu'_{p_{ijm}})^{\lambda_{ijm}} \right) \tag{B66a}$$

or

$$= \prod_m \left(\sum_j C_{jm} \pi_i (\mu'_{p_{ijm}})^{\lambda_{ijm}} \right) . \tag{B66b}$$

As an example, we compute $\varkappa_3\varkappa_2$. We already know $\varkappa_3$ in terms of parent moments from Eq. (B63). The partition of 2 is

$$\{2,\ 1+1\}$$

or

$$\{2^1,\ 1^2\}\ .$$

The term corresponding to the combination 2^1 is

$$\frac{2!(-1)^{(1-1)}(1-1)!}{(2!)^1(1!)}(\mu_2')^1$$

$$= \mu_2'\ .$$

The term corresponding to 1^2 is

$$\frac{2!(-1)^{(2-1)}(2-1)!}{(1!)^2(2!)}(\mu_1')^2$$

$$= -\mu_1'^2$$

Therefore

$$\kappa_2 = \mu_2' - \mu_1'^2\ . \tag{B67}$$

From Eqs. (B63), and (B67), we know that

$$\kappa_3\kappa_2 = (\mu_3' - 3\mu_2'\mu_1' + 2\mu_1'^3)(\mu_2' - \mu_1'^2)$$

$$= \mu_3'\mu_2' - \mu_3'\mu_1'^2 - 3\mu_2'^2\mu_1' + 5\mu_2'\mu_1'^3 - 2\mu_1'^5\ . \tag{B68}$$

Now that we know $\kappa_3\kappa_2$ in terms of parent moments, we can use Eqs. (B30) and (B53a) to find the k-statistic k_{32}. That is,

$$k_{32} = U(\kappa_3 \kappa_2)$$

$$= U(\mu_3'\mu_2') - U(\mu_3'\mu_1'^2) - 3U(\mu_2'^2\mu_1') + 5U(\mu_2'\mu_1'^3) - 2U(\mu_1'^5)$$

$$= \frac{[32]}{M^{[2]}} - \frac{[31^2]}{M^{[3]}} - \frac{3[2^2 1]}{M^{[3]}} + \frac{5[21^3]}{M^{[4]}} - \frac{2[1^5]}{M^{[5]}} \quad . \tag{B69}$$

In order to express a given k-statistic in closed form, we must first change Eqs. (B66a) and (B66b) from a product of sums to a sum of products. In order to accomplish this, we must change our indexing system somewhat. For example, it is clear from Eqs. (B64b) and (B66b) that we could represent κ_3 and κ_2 as

$$\kappa_3 = c_{11}\mu_3' + c_{21}\mu_2'\mu_1' + c_{31}\mu_1'^3$$

$$\kappa_2 = c_{12}\mu_2' + c_{22}\mu_1'^2$$

and $\kappa_3\kappa_2$ as

$$\begin{aligned}\kappa_3\kappa_2 &= c_{11}c_{12}\mu_3'\cdot\mu_2' + c_{11}c_{22}\mu_3'\cdot\mu_1'^2 \\ &+ c_{21}c_{12}\mu_2'\mu_1'\cdot\mu_2' + c_{21}c_{22}\mu_2'\mu_1'\cdot\mu_1'^2 \\ &+ c_{31}c_{12}\mu_1'^3\cdot\mu_2' + c_{31}c_{22}\mu_1'^3\cdot\mu_1'^2 \quad .\end{aligned} \tag{B70}$$

In Eq. (B70), the first index of C_{jm} labels the j-th combination of the m-th partition. We could, however, allow j to lable the j-th <u>combination pair</u> of the partitions 3 and 2. The partitions of 3 and 2 are

$$\{3,\ 2+1,\ 1+1+1\} \text{ and } \{2,\ 1+1\}$$

or

$$\{3^1,\ 2^1 1^1,\ 1^3\} \quad \text{and} \quad \{2^1,\ 1^2\} \quad .$$

The corresponding set of combination pairs is

$$\{3^1 \cdot 2^1,\ 3^1 \cdot 1^2,\ 2^1 1^1 \cdot 2^1,\ 2^1 1^1 \cdot 1^2,\ 1^3 \cdot 2^1,\ 1^3 \cdot 1^2\},$$

If j is the index for combination pairs, $\varkappa_3 \varkappa_2$ would be represented as

$$\varkappa_3 \varkappa_2 = c_{11} c_{12} \mu'_3 \cdot \mu'_2 + c_{21} c_{22} \mu'_3 \cdot \mu'^2_1$$

$$+ c_{31} c_{32} \mu'_2 \mu'_1 \cdot \mu'_2 + c_{41} c_{42} \mu'_2 \mu'_1 \cdot \mu'^2_1$$

$$+ c_{51} c_{52} \mu'^3_1 \cdot \mu'_2 + c_{61} c_{62} \mu'^3_1 \cdot \mu'^2_1 \ .$$

For a product of three cumulants, the equivalent sum could be over combination triplets; in general, a cumulant product could be expressed as a sum over a set of combination multiplets. Using this new notation, any cumulant product can be expressed as

$$\varkappa_{r_1} \varkappa_{r_2 \ldots} = \sum_j \prod_m \left(C_{jm} \prod_i (\mu'_{p_{ijm}})^{\lambda_{ijm}} \right) \ . \tag{B71}$$

Because multiplication is associative

$$\varkappa_{r_1} \varkappa_{r_2 \ldots} = \sum_j \left(\prod_m C_{jm} \right) \prod_{m,i} (\mu'_{p_{ijm}})^{\lambda_{ijm}} \tag{B72}$$

$$\varkappa_{r_1} \varkappa_{r_2 \ldots} = \sum_j \left(\prod_m \frac{r_m! (-1)^{\rho_{jm}-1} (\rho_{jm}-1)!}{\prod_i \{(p_{ijm})!^{\lambda_{ijm}} (\lambda_{ijm})!\}} \right) \prod_{m,i} \left(\mu'_{p_{ijm}} \right)^{\lambda_{ijm}} \ , \tag{B73}$$

or employing Wishart's notation as in Eq. (B51), Section 5,

$$\varkappa_r \varkappa_s \ldots = r!s!\ldots \sum \frac{(-1)^{\Sigma(\rho-1)} \pi \{(\rho-1)!\}}{\pi\{(\lambda_1!\lambda_2!\ldots)\}} \prod \left\{ \left(\frac{\mu'_{p_1}}{p_1!} \right)^{\lambda_1} \left(\frac{\mu_{p_2}}{p_2!} \right)^{\lambda_2} \ldots \right\} .$$

From Eq. (B73), we can easily find that the k-statistic corresponding to $\varkappa_{r_1} \varkappa_{r_2} \ldots$ is

$$k_{r_1 r_2 \ldots} = \sum_j \left(\prod_m \frac{r_m! (-1)^{\rho_{jm}-1} (\rho_{jm}-1)!}{\pi_i \{(p_{ijm})!^{\lambda_{ijm}} (\lambda_{ijm})!\}} \right) \frac{[\pi_{m,i} \, p_{ijm}^{\lambda_{ijm}}]}{M^{[\Sigma_m \rho_{jm}]}} \tag{B74}$$

because we know from Eq. (B30) that

$$U\left(\prod_{m,i} (\mu'_{p_{ijm}})^{\lambda_{ijm}} \right) = \frac{[\pi_{m,i} \, p_{ijm}^{\lambda_{ijm}}]}{M^{[\Sigma_m \rho_{jm}]}} .$$

Using Wishart's notation, the k statistic $k_{rs\ldots}$ can be expressed as

$$k_{rs\ldots} =$$

$$\sum \frac{(-1)^{\Sigma(\rho-1)} \pi\{(\rho-1)!\}}{\pi\{\lambda_1!\lambda_2!\ldots\}} \frac{r!s!\ldots}{\pi\{(p_1!)^{\lambda_1}(p_2!)^{\lambda_2}\ldots\}} \frac{[\pi(p_1^{\lambda_1} p_2^{\lambda_2}\ldots)]}{M^{[\Sigma\rho]}} .$$

Let us, for example consider computing k_{32}, the unbiased estimator of $\varkappa_3 \varkappa_2$, in terms of augmented symmetric functions. We apply Eq. (B74) to this problem and let $r_1 = 3$ and $r_2 = 2$. Therefore

$$k_{32} =$$

$$\sum_j \frac{3!(-1)^{\rho_{j1}-1}(\rho_{j1}-1)!}{\pi_i \{(p_{ij1})!^{\lambda_{ij1}}(\lambda_{ij1})!\}} \frac{2!(-1)^{\rho_{j2}-1}(\rho_{j2}-1)!}{\pi_i \{(p_{ij2})!^{\lambda_{ij2}}(\lambda_{ij2})!\}} \frac{[\pi_i \, p_{ij1}^{\lambda_{ij1}} p_{ij2}^{\lambda_{ij2}}]}{M^{[\rho_{j1}+\rho_{j2}]}} . \tag{B75}$$

We recall that the partitions of 3 and 2 are

$$\{3^1,\ 2^1 1^1,\ 1^3\} \text{ and } \{2^1,\ 1^2\}\ ,$$

and the set of combination pairs that Eq.(B75) is summed over is therefore

$$\{3^1 \cdot 2^1,\ 3^1 \cdot 1^2,\ 2^1 1^1 \cdot 2^1,\ 2^1 1^1 \cdot 1^2,\ 1^3 \cdot 2^1,\ 1^3 \cdot 1^2\}\ .$$

The term corresponding to $3^1 \cdot 2^1$ is

$$\frac{3!(-1)^{\rho_{11}-1}(\rho_{11}-1)!}{\pi_i \{(p_{i11})!^{\lambda_{i11}}(\lambda_{i11})!\}} \frac{2!(-1)^{\rho_{12}-1}(\rho_{12}-1)!}{\pi_i \{(p_{i12})!^{\lambda_{i12}}(\lambda_{i12})!\}} \frac{[\pi_i\, p_{i11}^{\lambda_{i11}} p_{i12}^{\lambda_{i12}}]}{M^{[\rho_{11}+\rho_{12}]}}$$

$$= \frac{3!(-1)^{(1-1)}(1-1)!}{(3!)^1\ (1!)} \frac{2!(-1)^{(1-1)}(1-1)!}{(2!)^1\ (1!)} \frac{[3^1 \cdot 2^1]}{M^{[1+1]}}$$

$$= [32]/M^{[2]}\ .$$

The term corresponding to $3^1 1^2$ is

$$\frac{3!(-1)^{\rho_{21}-1}(\rho_{21}-1)!}{\pi_i \{(p_{i21})!^{\lambda_{i21}}(\lambda_{i21})!\}} \frac{2!(-1)^{\rho_{22}-1}(\rho_{22}-1)!}{\pi_i \{(p_{i22})!^{\lambda_{i22}}(\lambda_{i22})!\}} \frac{[\pi_i\ p_{i21}^{\lambda_{i21}} p_{i22}^{\lambda_{i22}}]}{M^{[\rho_{21}+\rho_{22}]}}$$

$$= \frac{3!(-1)^{(1-1)}(1-1)!}{(3!)^1 (1!)} \frac{2!(-1)^{(2-1)}(2-1)!}{(1!)^2 (2!)} \frac{[3^1 \cdot 1^2]}{M^{[1+2]}}$$

$$= -\ [31^2]/M^{[3]}\ .$$

The term corresponding to $2^1 1^1 \cdot 2^1$ is

$$\frac{3!(-1)^{(2-1)}(2-1)!}{\{(2!)^1(1!)\}\{(1!)^1(1!)\}} \quad \frac{2!(-1)^{(1-1)}(1-1)!}{(2!)^1(1!)} \quad \frac{[2^1 1^1 \cdot 2^1]}{M^{[2+1]}}$$

$$= -3[2^2 1]/M^{[3]} \quad .$$

The term for $2^1 1^1 \cdot 1^2$ is

$$\frac{3!(-1)^{(2-1)}(2-1)!}{\{(2!)^1(1!)\}\{(1!)^1(1!)\}} \quad \frac{2!(-1)^{(2-1)}(2-1)!}{(1!)^2(2!)} \quad \frac{[2^1 1^1 \cdot 1^2]}{M^{[2+2]}}$$

$$= 3[21^3]/M^{[4]}.$$

The term for the combination pair $1^3 \cdot 2^1$ is

$$\frac{3!(-1)^{(3-1)}(3-1)!}{(1!)^3(3!)} \quad \frac{2!(-1)^{(1-1)}(1-1)!}{(2!)^1(1!)} \quad \frac{[1^3 \cdot 2^1]}{M^{[3+1]}}$$

$$= 2[21^3]/M^{[4]} \quad .$$

The last term, which corresponds to the combination pair $1^3 \cdot 1^2$, is

$$\frac{3!(-1)^{(3-1)}(3-1)!}{(1!)^3(3!)} \quad \frac{2!(-1)^{(2-1)}(2-1)!}{(1!)^2(2!)} \quad \frac{[1^3 \cdot 1^2]}{M^{[3+2]}}$$

$$= -2[1^5]/M^{[5]} \quad .$$

Therefore, we know that

$$k_{32} = \frac{[32]}{M^{[2]}} - \frac{[31^2]}{M^{[3]}} - \frac{3[2^2 1]}{M^{[3]}} + \frac{3[21^3]}{M^{[4]}} + \frac{2[21^3]}{M^{[4]}} - \frac{2[1^5]}{M^{[5]}}$$

$$= \frac{[32]}{M^{[2]}} - \frac{[31^2]}{M^{[3]}} - \frac{3[2^2 1]}{M^{[3]}} + \frac{5[21^3]}{M^{[4]}} - \frac{2[1^5]}{M^{[5]}} \quad ,$$

which agrees with the expression for k_{32} obtained in Eq. (B69).

11. Another Application of Cumulants

In Appendix A, we found that in order to compute the parent moments μ_2, μ_4, μ_6 and μ_8, it was convenient to define $G^{(r)}(t,1)$ in Eq. (A13) as

$$G^{(r)}(t,1) = \left(\frac{\partial}{\partial z}\right)^r \exp[F(t,z)]\Big|_{z=1}$$

Sections 4 and 7 of Appendix A were spent in finding $G^{(r)}(t,1)$ in terms of $F^{(r)}(t,1)$ for r ranging over the integers from 1 to 8. These tedious calculations can be circumvented however, by observing that μ'_r is related to $\varkappa_r$ in a way similar to that in which $G^{(r)}(t,1)$ is related to $F^{(r)}(t,1)$. From Eqs. (B37) and (B39), we recall that

$$\mu'_r = \left(-i \frac{d}{dt}\right)^r \phi(t)\Big|_{t=0}$$

$$\varkappa_r = \left(-i \frac{d}{dt}\right)^r \log \phi(t)\Big|_{t=0} \quad .$$

We can define $\rho(t) \equiv \log \phi(t)$ and make the change of variables $x = it$, to find that

$$\mu_r' = \left(\frac{d}{dx}\right)^r \exp[\rho(x)]\Big|_{x=0} \tag{B76a}$$

$$\kappa_r = \left(\frac{d}{dx}\right)^r \rho(x)\Big|_{x=0} \quad . \tag{B76b}$$

We would expect then that $G^{(r)}(t,1)$ can be expressed in terms of $F^{(r)}(t,1)$ in the same way that μ_r' is expressed in terms of κ_r. For instance, from the fact that μ_4' can be expressed in terms of cumulants as

$$\mu_4' = \kappa_4 + 4\kappa_3\kappa_1 + 3\kappa_2^2 + 6\kappa_2\kappa_1^2 + \kappa_1^4$$

we know that

$$G^{(4)}(1,t) = F^{(4)}(1,t) + 4F^{(3)}(1,t)F^{(1)}(1,t) + 3[F^{(2)}(1,t)]^2$$
$$+ 6F^{(2)}(1,t)[F^{(1)}(1,t)]^2 + [F^{(1)}(1,t)]^4 \ ,$$

as is confirmed by Eq. (A14d). Therefore, the method used in expressing moments in terms of cumulants can also be used to express $G^{(r)}(1,t)$ in terms of $F^{(r)}(1,t)$.

APPENDIX C

VARIANCES AND UNBIASED ESTIMATORS OF αt AND βt

1. Introduction

The purpose of this section is to give detailed derivations of quantities mentioned in the main body of the paper. Here we derive the unbiased estimators of αt and βt, the variances of $\widehat{\alpha t}$ and $\widehat{\beta t}$, and the unbiased estimators of these variances.

2. Unbiased Estimators of αt and βt

Equation (36a) gives αt in terms of parent moments

$$\alpha t = \frac{1}{6}[4\mu_2 + 3(\mu_2)^2 - \mu_4] \quad .$$

Algorithm B1 given in Section 6 of Appendix B shows how to find the unbiased estimator of a population value such as αt. First, we find αt in terms of cumulant products. Equations (B48a) and (B48c) give the parent moments μ_2 and μ_4 in terms of cumulants:

$$\mu_2 = \varkappa_2$$

$$\mu_4 = \varkappa_4 + 3\varkappa_2^2 \quad .$$

Therefore, αt can be expressed as

$$\alpha t = \frac{1}{6}[4(\varkappa_2) + 3(\varkappa_2)^2 - (\varkappa_4 + 3\varkappa_2^2)]$$

$$= \frac{1}{6}[4\varkappa_2 - \varkappa_4] \quad . \tag{C1}$$

The unbiased estimator of αt is then, by Eq. (B53a),

$$\widehat{\alpha t} = \frac{1}{6}[4\,\widehat{\varkappa}_2 - \widehat{\varkappa}_4]$$

$$= \frac{1}{6}[4k_2 - k_4] \quad . \tag{C2}$$

Because k_2 and k_4 are of orders 2 and 4 respectively, tables of orders 2 and 4 are necessary for finding the k-statistics in terms of augmented symmetric functions. Using Tables B3 and B4, we find that

$$\hat{\alpha t} = \frac{1}{6}\{4(-\frac{[1^2]}{M^{[2]}} + \frac{[2]}{M})$$

$$- (-\frac{6[1^4]}{M^{[4]}} + \frac{12[21^2]}{M^{[3]}} - \frac{3[2^2]}{M^{[2]}} - \frac{4[31]}{M^{[2]}} + \frac{[4]}{M})\} . \qquad (C3)$$

From the second and fourth order augmented symmetric function/power sum Tables B2 and B5, and Algorithm B1, we see that

$$\hat{\alpha t} = \frac{1}{6}\{ - \frac{4}{M^{[2]}}(-s_2) + \frac{4}{M}(s_2) + \frac{6}{M^{[4]}}(-6s_4 + 3s_2^2)$$

$$- \frac{12}{M^{[3]}}(2s_4 - s_2^2) + \frac{3}{M^{[2]}}(-s_4 + s_2^2) + \frac{4}{M^{[2]}}(-s_4) - \frac{(s_4)}{M}\}$$

$$= \frac{1}{6}\{\frac{4s_2}{M^{[2]}} + \frac{4s_2}{M} - \frac{36s_4}{M^{[4]}} + \frac{18s_2^2}{M^{[4]}} - \frac{24s_4}{M^{[3]}} + \frac{12s_2^2}{M^{[3]}} - \frac{7s_4}{M^{[2]}} + \frac{3s_2^2}{M^{[2]}} - \frac{s_4}{M}\}$$

$$= \frac{1}{6}\{4(\frac{1}{M} + \frac{1}{M^{[2]}})s_2 + 3(\frac{1}{M^{[2]}} + \frac{4}{M^{[3]}} + \frac{6}{M^{[4]}})s_2^2$$

$$- (\frac{1}{M} + \frac{7}{M^{[2]}} + \frac{24}{M^{[3]}} + \frac{36}{M^{[4]}})s_4\}$$

$$= \frac{1}{6}\{4(\frac{1}{M} + \frac{1}{M^{[2]}})Mm_2 + 3(\frac{1}{M^{[2]}} + \frac{4}{M^{[3]}} + \frac{6}{M^{[4]}})M^2m_2^2$$

$$- (\frac{1}{M} + \frac{7}{M^{[2]}} + \frac{24}{M^{[3]}} + \frac{36}{M^{[4]}})Mm_4\}$$

$$= \frac{1}{6}\{\frac{4M}{M-1}m_2 + 3M(\frac{1}{(M-1)} + \frac{4}{(M-1)^{[2]}} + \frac{6}{(M-1)^{[3]}})m_2^2$$

$$- (1 + \frac{7}{(M-1)} + \frac{24}{(M-1)^{[2]}} + \frac{36}{(M-1)^{[3]}})m_4\} . \qquad (C4)$$

Similarly, $\hat{\beta t}$ can be found in terms of the sample moments. From Eq. (36b), we know that

$$\beta t = \frac{1}{24}\,[\mu_4 - 3\mu_2^2 - \mu_2] \quad .$$

In terms of cumulants, βt is

$$\beta t = \frac{1}{24}\,[\kappa_4 + 3\kappa_2^2 - 3\kappa_2^2 - \kappa_2]$$

$$= \frac{1}{24}\,[\kappa_4 - \kappa_2] \quad . \tag{C5}$$

Again we use Eq. (53a) to find the expectation values of the cumulants:

$$\hat{\beta t} = \frac{1}{24}\,[\hat{\kappa}_4 - \hat{\kappa}_2]$$

$$= \frac{1}{24}\,[k_4 - k_2] \quad . \tag{C6}$$

We already know k_4 and k_2 in terms of augmented symmetric functions from calculating $\hat{\alpha t}$, so that

$$\hat{\beta t} = \frac{1}{24}\left\{\left(-\frac{6[1^4]}{M^{[4]}} + \frac{12[21^2]}{M^{[3]}} - \frac{3[2^2]}{M^{[2]}} - \frac{4[31]}{M^{[2]}} + \frac{[4]}{M}\right) - \left(-\frac{[1^2]}{M^{[2]}} + \frac{[2]}{M}\right)\right\}$$

$$= \frac{1}{24}\left\{-\frac{6[1^4]}{M^{[4]}} + \frac{12[21^2]}{M^{[3]}} - \frac{3[2^2]}{M^{[2]}} - \frac{4[31]}{M^{[2]}} + \frac{[4]}{M} + \frac{[1^2]}{M^{[2]}} - \frac{[2]}{M}\right\} .$$

Tables B2 and B5, and algorithm B1 show that $\hat{\beta t}$ can be expressed as

$$\hat{\beta}t = \frac{1}{24}\{ -\frac{6(-6s_4+3s_2^2)}{M^{[4]}} + \frac{12}{M^{[3]}}(2s_4 - s_2^2) - \frac{3}{M^{[2]}}(-s_4+s_2^2)$$

$$- \frac{4(-s_4)}{M^{[2]}} + \frac{(s_4)}{M} + \frac{(-s_2)}{M^{[2]}} - \frac{(s_2)}{M} \}$$

$$= \frac{1}{24}\{ (\frac{1}{M} + \frac{4}{M^{[2]}} + \frac{3}{M^{[2]}} + \frac{24}{M^{[3]}} + \frac{36}{M^{[4]}})\, s_4$$

$$+ (-\frac{3}{M^{[2]}} - \frac{12}{M^{[3]}} - \frac{18}{M^{[4]}})\, s_2^2 - (\frac{1}{M^{[2]}} + \frac{1}{M})\, s_2$$

$$= \frac{1}{24}\{ (\frac{1}{M} + \frac{7}{M^{[2]}} + \frac{24}{M^{[3]}} + \frac{36}{M^{[4]}})\, Mm_4$$

$$- (\frac{3}{M^{[2]}} + \frac{12}{M^{[3]}} + \frac{18}{M^{[4]}})\, M^2 m_2^2 - (\frac{1}{M^{[2]}} + \frac{1}{M})\, Mm_2 \}$$

$$= \frac{1}{24}\{ (1 + \frac{7}{(M-1)} + \frac{24}{(M-1)^{[2]}} + \frac{36}{(M-1)^{[3]}})\, m_4$$

$$- 3M(\frac{1}{(M-1)} + \frac{4}{(M-1)^{[2]}} + \frac{6}{(M-1)^{[3]}})\, m_2^2 - \frac{M}{(M-1)} m_2 \} \quad . \tag{C7}$$

We can also express $\hat{\alpha}t$ and $\hat{\beta}t$, given in Eqs. (C4) and (C7), as

$$\hat{\alpha}t = R_\alpha m_2 + S_\alpha m_2^2 + T_\alpha m_4 \tag{C8a}$$

$$\hat{\beta}t = R_\beta m_2 + S_\beta m_2^2 + T_\beta m_4 \tag{C8b}$$

where

$$R_\alpha = \frac{2M}{3(M-1)} \tag{C9a}$$

$$S_\alpha = \frac{M}{2}(\frac{1}{(M-1)} + \frac{4}{(M-1)^{[2]}} + \frac{6}{(M-1)^{[3]}}) \tag{C9b}$$

$$T_\alpha = -\frac{1}{6}(1 + \frac{7}{(M-1)} + \frac{24}{(M-1)^{[2]}} + \frac{36}{(M-1)^{[3]}}) \tag{C9c}$$

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STATISTICS OF 1-DIMENSIONAL ATOM MOTION WITH NEXT-NEAREST NEIGH--ETC(U)
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$$R_\beta = -\frac{M}{24(M-1)}$$

$$S_\beta = -\frac{M}{8}\left(\frac{1}{(M-1)} + \frac{4}{(M-1)^{[2]}} + \frac{6}{(M-1\right.$$

$$T_\beta = \frac{1}{24}\left(1 + \frac{7}{(M-1)} + \frac{24}{(M-1)^{[2]}} + \right.$$

3. Variances of $\hat{\alpha t}$ and $\hat{\beta t}$

Equation (51a) gives the variance

$$\mathrm{var}\ \hat{\alpha t} = \langle (\hat{\alpha t})^2 \rangle - (\alpha t)$$

We already know $\hat{\alpha t}$ from Eq. (C2); the squar

$$(\hat{\alpha t})^2 = \frac{1}{36}\left[16k_2^2 - 8k_4k_2 + k_4^2\right] .$$

It is not immediately obvious how we can fi $(\hat{\alpha t})^2$ from Eq. (C11). However, the k-statis can be reduced to a more pliable state by r a sum of individual k-statistics. Consulti Appendix F, we find that [11]

$$k_4^2 = \frac{k_8}{M} + \frac{16k_{62}}{(M-1)} + \frac{48k_{53}}{(M-1)} + \frac{(M+33)}{(M-1)}$$

$$+ \frac{144\ M}{(M-1)^{[2]}}\,k_{322} + \frac{24M(M+1)}{(M-1)^{[3]}}\,k$$

$$k_4k_2 = \frac{k_6}{M} + \frac{(M+7)}{(M-1)}\,k_{42} + \frac{6}{(M-1)}k_{33}$$

$$k_2^2 = \frac{k_4}{M} + \frac{(M+1)}{(M-1)}\,k_{22} .$$

We can now write

$$(\hat{\alpha t})^2 = \frac{1}{36}\left\{ \frac{k_8}{M} + \frac{16k_{62}}{(M-1)} + \frac{48k_{53}}{(M-1)} + \frac{(M+33)}{(M-1)} k_{44} + \frac{72M}{(M-1)^{[2]}} k_{422} \right.$$

$$+ \frac{144M}{(M-1)^{[2]}} k_{332} + \frac{24M(M+1)}{(M-1)^{[3]}} k_{2222}$$

$$\left. - 8\left(\frac{k_6}{M} + \frac{(M+7)}{(M-1)} k_{42} + \frac{6k_{33}}{(M-1)} \right) + 16\left(\frac{k_4}{M} + \frac{(M+1)}{(M-1)} k_{22} \right) \right\} .$$

Performing the proper multiplications, it appears that

$$(\hat{\alpha t})^2 = \frac{1}{36}\left\{ \frac{k_8}{M} + \frac{16k_{62}}{(M-1)} + \frac{48k_{53}}{(M-1)} + \frac{(M+33)}{(M-1)} k_{44} + \frac{72M}{(M-1)^{[2]}} k_{422} \right.$$

$$+ \frac{144M}{(M-1)^{[2]}} k_{332} + \frac{24M(M+1)}{(M-1)^{[3]}} k_{2222} - \frac{8k_6}{M} - \frac{8(M+7)}{(M-1)} k_{42}$$

$$\left. - \frac{48k_{33}}{(M-1)} + \frac{16k_4}{M} + \frac{16(M+1)}{(M-1)} k_{22} \right\} . \tag{C13}$$

By Eqs. (B53a) and (42), however,

$$\langle (\hat{\alpha t})^2 \rangle = \frac{1}{36}\left\{ \frac{\kappa_8}{M} + \frac{16\kappa_6\kappa_2}{(M-1)} + \frac{48\kappa_5\kappa_3}{(M-1)} + \frac{(M+33)}{(M-1)} \kappa_4^2 + \frac{72M}{(M-1)^{[2]}} \kappa_4\kappa_2^2 \right.$$

$$+ \frac{144M}{(M-1)^{[2]}} \kappa_3^2\kappa_2 + \frac{24M(M-1)}{(M-1)^{[3]}} \kappa_2^4 - \frac{8\kappa_6}{M} - \frac{8(M+7)}{(M-1)} \kappa_4\kappa_2$$

$$\left. - \frac{48\kappa_3^2}{(M-1)} + \frac{16\kappa_4}{M} + \frac{16(M+1)}{(M-1)}\kappa_2^2 \right\} . \tag{C14}$$

According to Eqs. (B49a)-(B49g), the odd cumulants involve moment products that must include at least one odd moment as a factor. Because all odd parent moments as defined by Eq. (29) are zero, odd cumulants are also zero. Therefore, from Eqs. (51a) and (C14), we know that

$$\sigma_{\alpha t}{}^2 \equiv \mathrm{var}\ \hat{\alpha t}$$

$$= \frac{1}{36}\left\{ \frac{\kappa_8}{M} + \frac{16\kappa_6\kappa_2}{(M-1)} + \frac{(M+33)}{(M-1)}\kappa_4^2 + \frac{72M}{(M-1)^{[2]}}\kappa_4\kappa_2^2 \right.$$

$$+ \frac{24M(M+1)}{(M-1)^{[3]}}\kappa_2^4 - \frac{8\kappa_6}{M} - \frac{8(M+7)}{(M-1)}\kappa_4\kappa_2$$

$$\left. + \frac{16\kappa_4}{M} + \frac{16(M+1)}{(M-1)}\kappa_2^2 \right\} - (\alpha t)^2 \ . \qquad \text{(C15)}$$

Equation (51b) gives the variances of $\hat{\beta t}$ as

$$\mathrm{var}\ \hat{\beta t} = \langle (\hat{\beta t})^2 \rangle - (\beta t)^2 \ .$$

We already know $\hat{\beta t}$ from Eq. (C6); the square of this quantity is

$$(\hat{\beta t})^2 = \frac{1}{576}\left[k_4^2 - 2k_4k_2 + k_2^2\right] . \qquad \text{(C16)}$$

Substituting Eqs. (C12a)-(C12c) into Eq. (C16), we find that

$$(\hat{\beta t})^2 = \frac{1}{576}\left\{ \frac{k_8}{M} + \frac{16}{(M-1)}k_{62} + \frac{48k_{53}}{(M-1)} + \frac{(M+33)}{(M-1)}k_{44} + \frac{72M}{(M-1)^{[2]}}k_{422} \right.$$

$$+ \frac{144M}{(M-1)^{[2]}}k_{332} + \frac{24M(M+1)}{(M-1)^{[3]}}k_{2222} - \frac{2k_6}{M} - \frac{2(M+7)}{(M-1)}k_{42}$$

$$\left. - \frac{12}{(M-1)}k_{33} + \frac{k_4}{M} + \frac{(M+1)}{(M-1)}k_{22} \right\} . \qquad \text{(C17)}$$

By Eqs (B53a) and (51b), the variance of $\hat{\beta t}$ is then

$$\sigma_{\beta t}^{\ 2} \equiv \operatorname{var} \hat{\beta t}$$

$$= \frac{1}{576} \{ \frac{\kappa_8}{M} + \frac{16\kappa_6\kappa_2}{(M-1)} + \frac{(M+33)}{(M-1)} \kappa_4^2 + \frac{72M}{(M-1)^{[2]}} \kappa_4\kappa_2^2$$

$$+ \frac{24M(M+1)}{(M-1)^{[3]}} \kappa_2^4 - \frac{2\kappa_6}{M} - \frac{2(M+7)}{(M-1)} \kappa_4\kappa_2 + \frac{\kappa_4}{M}$$

$$+ \frac{(M+1)}{(M-1)} \kappa_2^2 \} - (\beta t)^2 \quad . \qquad \text{(C18)}$$

4. <u>First Order Approximations for var $\hat{\alpha t}$ and var $\hat{\beta t}$</u>

From Eqs. (C1) and (C15) we know that the variance of $\hat{\alpha t}$ can be written in terms of cumulants as

$$\operatorname{var} \hat{\alpha t} = \frac{1}{36} [\frac{\kappa_8}{M} + \frac{16\kappa_6\kappa_2}{(M-1)} + \frac{(M+33)}{(M-1)} \kappa_4^2 + \frac{72M}{(M-1)^{[2]}} \kappa_4\kappa_2^2$$

$$+ \frac{24M(M+1)}{(M-1)^{[3]}} \kappa_2^4 - \frac{8\kappa_6}{M} - \frac{8(M+7)}{(M-1)} \kappa_4\kappa_2 + \frac{16\kappa_4}{M} + \frac{16(M+1)}{(M-1)} \kappa_2^2]$$

$$- [\frac{1}{6} (4\kappa_2 - \kappa_4)]^2$$

$$= \frac{1}{36} [\frac{\kappa_8}{M} + \frac{16\kappa_6\kappa_2}{(M-1)} + \frac{(M+33)}{(M-1)} \kappa_4^2 + \frac{72M}{(M-1)^{[2]}} \kappa_4\kappa_2^2$$

$$+ \frac{24M(M+1)}{(M-1)^{[3]}} \kappa_2^4 - \frac{8\kappa_6}{M} - \frac{8(M+7)}{(M-1)} \kappa_4\kappa_2 + \frac{16\kappa_4}{M} + \frac{16(M+1)}{(M-1)} \kappa_2^2$$

$$- 16\kappa_2^2 + 8\kappa_2\kappa_4 - \kappa_4^2] \ .$$

To first order in 1/M, var $\hat{\alpha t}$ is then

$$\mathrm{var}\ \hat{\alpha t} \simeq \frac{1}{36M}(\kappa_8 + 16\kappa_6\kappa_2 + 33\kappa_4^2 + 72\kappa_4\kappa_2^2 + 24\kappa_2^4 - 8\kappa_6$$

$$- 56\kappa_4\kappa_2 + 16\kappa_4 + 16\kappa_2^2) . \qquad \text{(C19)}$$

We can substitute Eqs. (60a)-(60d) into Eq. (C19) and find var $\hat{\alpha t}$ in terms of parent moments:

$$\mathrm{var}\ \hat{\alpha t} \simeq \frac{1}{36M}[(\mu_8 - 28\mu_6\mu_2 - 35\mu_4^2 + 420\mu_4\mu_2^2 - 630\mu_2^4)$$

$$+ 16(\mu_6 - 15\mu_4\mu_2 + 30\mu_2^3)\mu_2 + 33(\mu_4 - 3\mu_2^2)^2$$

$$+ 72(\mu_4 - 3\mu_2^2)\mu_2^2 + 24\mu_2^4 - 8(\mu_6 - 15\mu_4\mu_2 + 30\mu_2^3)$$

$$- 56(\mu_4 - 3\mu_2^2)\mu_2^2 + 16(\mu_4 - 3\mu_2^2) + 16\mu_2^2]$$

$$= \frac{1}{36M}[\mu_8 - 28\mu_6\mu_2 - 35\mu_4^2 + 420\mu_4\mu_2^2 - 630\mu_2^4$$

$$+ 16\mu_6\mu_2 - 240\mu_4\mu_2^2 + 480\mu_2^4$$

$$+ 33\mu_4^2 - 198\mu_4\mu_2^2 + 297\mu_2^4 + 72\mu_4\mu_2 - 216\mu_2^4$$

$$+ 24\mu_2^4 - 8\mu_6 + 120\mu_4\mu_2 - 240\mu_2^3$$

$$- 56\mu_4\mu_2 + 168\mu_2^3 + 16\mu_4 - 48\mu_2^2 + 16\mu_2^2]$$

$$= \frac{1}{36M}[\mu_8 - 12\mu_6\mu_2 - 2\mu_4^2 - 18\mu_4\mu_2^2 + 171\mu_2^4 + 136\mu_4\mu_2$$

$$- 72\mu_2^3 - 8\mu_6 + 16\mu_4 - 32\mu_2^2] . \qquad \text{(C20)}$$

Similarly, from Eqs. (C5) and (C18) we know that the variance of $\hat{\beta}t$ can be written in terms of cumulants as

$$\operatorname{var} \hat{\beta}t = \frac{1}{576} \left[\frac{\kappa_8}{M} + \frac{16\kappa_6\kappa_2}{(M-1)} + \frac{(M+33)}{(M-1)} \kappa_4^2 + \frac{72M}{(M-1)^{[2]}} \kappa_4\kappa_2^2\right.$$

$$+ \frac{24M(M+1)}{(M+1)^{[3]}} \kappa_2^4 - \frac{2\kappa_6}{M} - \frac{2(M+7)}{(M-1)} \kappa_4\kappa_2 + \frac{\kappa_4}{M}$$

$$\left. + \frac{(M+1)}{(M-1)} \kappa_2^2 \right] - \frac{1}{576} [\kappa_4 - \kappa_2]^2$$

$$= \frac{1}{576} \left[\frac{\kappa_8}{M} + \frac{16\kappa_6\kappa_2}{(M-1)} + \frac{(M+33)}{(M-1)} \kappa_4^2 + \frac{72M}{(M-1)^{[2]}} \kappa_4\kappa_2^2\right.$$

$$+ \frac{24M(M+1)}{(M+1)^{[3]}} \kappa_2^4 - \frac{2\kappa_6}{M} - \frac{2(M+7)}{(M-1)} \kappa_4\kappa_2 + \frac{\kappa_4}{M}$$

$$\left. + \frac{(M+1)}{(M-1)} \kappa_2^2 - \kappa_4^2 + 2\kappa_4\kappa_2 - \kappa_2^2 \right] .$$

To first order in $1/M$, var $\hat{\beta}t$ is then

$$\operatorname{var} \hat{\beta}t \simeq \frac{1}{576M} (\kappa_8 + 16\kappa_6\kappa_2 + 33\kappa_4^2 + 72\kappa_4\kappa_2^2 + 24\kappa_2^4 - 2\kappa_6$$

$$- 14\kappa_4\kappa_2 + \kappa_4 + \kappa_2^2) \quad . \tag{C21}$$

By substituting Eqs. (60a)-(60d) into Eq. (C21) we can find var $\hat{\beta}t$ in terms of the parent moments:

$$\operatorname{var} \hat{\beta}t \simeq \frac{1}{576M} [(\mu_8 - 28\mu_6\mu_2 - 35\mu_4^2 + 420\mu_4\mu_2^2 - 630\mu_2^4$$

$$+ 16(\mu_6 - 15\mu_4\mu_2 + 30\mu_2^3) \mu_2$$

$$+ 33(\mu_4 - 3\mu_2^2)^2 + 72(\mu_4 - 3\mu_2^2) \mu_2^2$$

$$+ 24\mu_2^4 - 2(\mu_6 - 15\mu_4\mu_2 + 30\mu_2^3)$$

$$- 14(\mu_4 - 3\mu_2^2)\mu_2 + (\mu_4 - 3\mu_2^2) + \mu_2^2 \,]$$

$$= \frac{1}{576M} [\mu_8 - 28\mu_6\mu_2 - 35\mu_4^2 + 420\mu_4\mu_2^2 - 630\mu_2^4$$

$$+ 16\mu_6\mu_2 - 240\mu_4\mu_2^2 + 480\mu_2^4$$

$$+ 33\mu_4^2 - 198\mu_4\mu_2^2 + 297\mu_2^4 + 72\mu_4\mu_2^2 - 216\mu_2^4$$

$$+ 24\mu_2^4 - 2\mu_6 + 30\mu_4\mu_2 - 60\mu_2^3$$

$$- 14\mu_4\mu_2 + 42\mu_2^3 + \mu_4 - 3\mu_2^2 + \mu_2^2]$$

$$= \frac{1}{576M} [\mu_8 - 12\mu_6\mu_2 - 2\mu_4^2 + 54\mu_4\mu_2^2 - 45\mu_2^4$$

$$- 2\mu_6 + 16\mu_4\mu_2 - 18\mu_2^3 + \mu_4 - 2\mu_2^2 \,] . \qquad \text{(C22)}$$

5. Unbiased Estimators of var $\hat{\alpha t}$ and var $\hat{\beta t}$

Equation (53a) gives the unbiased estimator of the variance of $\hat{\alpha t}$ as

$$U(\text{var } \hat{\alpha t}) = (\hat{\alpha t})^2 - U[(\alpha t)^2] \quad .$$

From Eq. (C1), we know that

$$\alpha t = \frac{1}{6} [4\kappa_2 - \kappa_4]$$

$$(\alpha t)^2 = \frac{1}{36} [16\kappa_2^2 - 8\kappa_4\kappa_2 + \kappa_4^2] \; . \qquad \text{(C23)}$$

Using Eq. (B53a) to derive the unbiased estimator of $(\alpha t)^2$, we find that

$$U[(\alpha t)^2] = \frac{1}{36} [16k_{22} - 8k_{42} + k_{44}] \quad . \qquad \text{(C24)}$$

Now we need only square the right hand side of Eq. (C8a) to obtain $(\widehat{\alpha t})^2$:

$$(\widehat{\alpha t})^2 = (R_\alpha m_2)^2 + 2(R_\alpha m_2)(S_\alpha m_2^2 + T_\alpha m_4) + (S_\alpha m_2^2 + T_\alpha m_4)^2$$

$$= R_\alpha^2 m_2^2 + 2R_\alpha S_\alpha m_2^3 + 2R_\alpha T_\alpha m_4 m_2 + S_\alpha^2 m_2^4$$

$$+ 2S_\alpha T_\alpha m_4 m_2^2 + T_\alpha^2 m_4^2 \quad . \tag{C25}$$

The coefficients R_α, S_α, and T_α are given by Eqs. (C9a)-(C9c). We combine Eqs. (53a), (C24), and (C25) and obtain

$$\widehat{\sigma_{\alpha t}^2} \equiv U(\text{var } \widehat{\alpha t})$$

$$= R_\alpha^2 m_2^2 + 2R_\alpha S_\alpha m_2^3 + 2R_\alpha T_\alpha m_4 m_2 + S_\alpha m_2^4 + 2S_\alpha T_\alpha m_4 m_2^2$$

$$+ T_\alpha^2 m_4^2 - \frac{4}{9} k_{22} + \frac{2}{9} k_{42} - \frac{1}{36} k_{44} \quad . \tag{C26}$$

Similarly, the unbiased estimator of var $\widehat{\beta t}$ can be found from Eq. (53b):

$$U(\text{var } \widehat{\beta t}) = (\widehat{\beta t})^2 - U[(\beta t)^2]$$

It follows from Eq. (C5) that

$$\beta t = \frac{1}{24} [\kappa_4 - \kappa_2]$$

$$(\beta t)^2 = \frac{1}{576} [\kappa_4^2 - 2\kappa_4\kappa_2 + \kappa_2^2] \quad . \tag{C27}$$

Using Eq. (B53a) to derive the unbiased estimator of $(\beta t)^2$, we note that

$$U[(\beta t)^2] = \frac{1}{576} [k_{44} - 2k_{42} + k_{22}] \quad . \tag{C28}$$

Squaring the right hand side of Eq. (C8b) it follows that $(\widehat{\beta t})^2$ is

$$(\widehat{\beta t})^2 = R_\beta^2 m_2^2 + 2R_\beta S_\beta m_2^3 + 2R_\beta T_\beta m_4 m_2 + S_\beta^2 m_2^4$$

$$+ 2S_\beta T_\beta m_4 m_2^2 + T_\beta^2 m_4^2 \quad . \tag{C29}$$

The coefficients R_β, S_β, and T_β are given by Eqs. (C10a)-C10c). We combine Eqs. (53b), (C28), and (C29), to find

$$\widehat{\sigma_{\beta t}^2} \equiv U(\mathrm{var}\ \hat{\beta}t)$$

$$= R_\beta^2 m_2^2 + 2R_\beta S_\beta m_2^3 + 2R_\beta T_\beta m_4 m_2 + S_\beta^2 m_2^2 + 2S_\beta T_\beta m_4 m_2^2$$

$$+ T_\beta^2 m_4^2 - \frac{1}{576} k_{22} + \frac{k_{42}}{288} - \frac{k_{44}}{576} \quad . \qquad \text{(C30)}$$

6. Evaluation of the k-statistics k_{22}, k_{42}, and k_{44}

Equations (C26) and (C30) give the unbiased estimators of $\sigma_{\alpha t}^2$ and $\sigma_{\beta t}^2$ in terms of sample moments and k-statistics. Here we find the relevant k-statistics in terms of sample moments also, so that the unbiased estimators of the variances can be easily evaluated.

First we calculate the k-statistic k_{22}. This k-statistic is of order 4; therefore we can find it in terms of augmented symmetric functions via Table B4, which is also of fourth order. That is,

$$k_{22} = \frac{[1^4]}{M^{[4]}} - \frac{2[21^2]}{M^{[3]}} + \frac{[2^2]}{M^{[2]}} \quad . \qquad \text{(C31)}$$

Applying Algorithm B1 to Eq. (C31) and Table B5, we arrive at

$$k_{22} = (-6s_4 + 3s_2^2)/M^{[4]} - 2(2s_4 - s_2^2)/M^{[3]} + (-s_4 + s_2^2)/M^{[2]}$$

$$= m_2^2 M^2 \left(\frac{1}{M^{[2]}} + \frac{2}{M^{[3]}} + \frac{3}{M^{[4]}}\right) - m_4 M \left(\frac{1}{M^{[2]}} + \frac{4}{M^{[3]}} + \frac{6}{M^{[4]}}\right) . \qquad \text{(C32)}$$

We can express the sixth order k-statistic k_{42} in terms of augmented symmetric functions by consulting the sixth order table in Appendix E and find that

$$k_{42} = \frac{6[1^6]}{M^{[6]}} - \frac{18[21^4]}{M^{[5]}} + \frac{15[2^2 1^2]}{M^{[4]}} + \frac{4[31^3]}{M^{[4]}} - \frac{3[2^3]}{M^{[3]}}$$

$$- \frac{4[321]}{M^{[3]}} - \frac{[41^2]}{M^{[3]}} + \frac{[42]}{M^{[2]}} \quad .$$

Applying Algorithm B1 to the augmented symmetric function/power sum tables of weight 6 given in Appendix E, it follows that

$$\begin{aligned}
k_{42} &= 6(-120s_6 + 90s_4s_2 + 40s_3^2 - 15s_2^3)/M^{[6]} \\
&\quad - 18(24s_6 - 18s_4s_2 - 8s_3^2 + 3s_2^3)/M^{[5]} \\
&\quad + 15(-6s_6 + 5s_4s_2 + 2s_3^2 - s_2^3)/M^{[4]} \\
&\quad + 4(-6s_6 + 3s_4s_2 + 2s_3^2)/M^{[4]} - 3(2s_6 - 3s_4s_2 + s_2^3)/M^{[3]} \\
&\quad - 4(2s_6 - s_4s_2 - s_3^2)/M^{[3]} - (2s_6 - s_4s_2)/M^{[3]} \\
&\quad + (-s_6 + s_4s_2)/M^{[2]} \\
&= - \frac{720s_6}{M^{[6]}} + \frac{540s_4s_2}{M^{[6]}} + \frac{240s_3^2}{M^{[6]}} - \frac{90s_2^3}{M^{[6]}} \\
&\quad - \frac{432s_6}{M^{[5]}} + \frac{324s_4s_2}{M^{[5]}} + \frac{144s_3^2}{M^{[5]}} - \frac{54s_2^3}{M^{[5]}} \\
&\quad - \frac{90s_6}{M^{[4]}} + \frac{75s_4s_2}{M^{[4]}} + \frac{30s_3^2}{M^{[4]}} - \frac{15s_2^3}{M^{[4]}} \\
&\quad - \frac{24s_6}{M^{[4]}} + \frac{12s_4s_2}{M^{[4]}} + \frac{8s_3^2}{M^{[4]}} - \frac{6s_6}{M^{[3]}} + \frac{9s_4s_2}{M^{[3]}} - \frac{3s_2^3}{M^{[3]}} \\
&\quad - \frac{8s_6}{M^{[3]}} + \frac{4s_4s_2}{M^{[3]}} + \frac{4s_3^2}{M^{[3]}} - \frac{2s_6}{M^{[3]}} + \frac{s_4s_2}{M^{[3]}} - \frac{s_6}{M^{[2]}} + \frac{s_4s_2}{M^{[2]}} \\
&= s_6\left(- \frac{720}{M^{[6]}} - \frac{432}{M^{[5]}} - \frac{90}{M^{[4]}} - \frac{24}{M^{[4]}} - \frac{8}{M^{[3]}} - \frac{6}{M^{[3]}} - \frac{2}{M^{[3]}} - \frac{1}{M^{[2]}}\right)
\end{aligned}$$

$$+ s_4 s_2 \left(\frac{540}{M^{[6]}} + \frac{324}{M^{[5]}} + \frac{75}{M^{[4]}} + \frac{12}{M^{[4]}} + \frac{4}{M^{[3]}} + \frac{9}{M^{[3]}} + \frac{1}{M^{[3]}} + \frac{1}{M^{[2]}} \right)$$

$$+ s_3^2 \left(\frac{240}{M^{[6]}} + \frac{144}{M^{[5]}} + \frac{30}{M^{[4]}} + \frac{8}{M^{[4]}} + \frac{4}{M^{[3]}} \right)$$

$$+ s_2^3 \left(- \frac{90}{M^{[6]}} - \frac{54}{M^{[5]}} - \frac{15}{M^{[4]}} - \frac{3}{M^{[3]}} \right)$$

$$= m_6 M \left(- \frac{1}{M^{[2]}} - \frac{16}{M^{[3]}} - \frac{114}{M^{[4]}} - \frac{432}{M^{[5]}} - \frac{720}{M^{[6]}} \right)$$

$$+ m_4 m_2 M^2 \left(\frac{1}{M^{[2]}} + \frac{14}{M^{[3]}} + \frac{87}{M^{[4]}} + \frac{324}{M^{[5]}} + \frac{540}{M^{[6]}} \right)$$

$$+ m_3^2 M^2 \left(\frac{4}{M^{[3]}} + \frac{38}{M^{[4]}} + \frac{144}{M^{[5]}} + \frac{240}{M^{[6]}} \right)$$

$$+ m_2^3 M^3 \left(- \frac{3}{M^{[3]}} - \frac{15}{M^{[4]}} - \frac{54}{M^{[5]}} - \frac{90}{M^{[6]}} \right) . \qquad \text{(C33)}$$

The k-statistic k_{44} is of eighth order. In Appendix E we have a twelth order table; an eighth order table is not available. We therefore use Algorithm B2 from Section 9 of Appendix B to find k_{44} in terms of augmented symmetric functions. This procedure gives

$$k_{44} = 36[1^8]/M^{[8]} - 144[21^6]/M^{[7]} + 180[2^2 1^4]/M^{[6]} - 72[2^3 1^2]/M^{[5]}$$

$$+ 9[2^4]/M^{[4]} + 48[31^5]/M^{[6]} - 96[321^3]/M^{[5]} + 24[32^2 1]/M^{[4]}$$

$$+ 16[3^2 1^2]/M^{[4]} - 12[41^4]/M^{[5]} + 24[421^2]/M^{[4]} - 6[42^2]/M^{[3]}$$

$$- 8[431]/M^{[3]} + [4^2]/M^{[2]} .$$

Applying Algorithm B1 to the augmented symmetric function/power sum tables of weight 8 given in Appendix E, yields

$$k_{44} = 36(-5040s_8 + 3360s_6s_2 + 2688s_5s_3 + 1260s_4^2 - 1260s_4s_2^2 - 1120s_3^2s_2 + 105s_2^4)/M^{[8]}$$

$$- 144(720s_8 - 480s_6s_2 - 384s_5s_3 - 180s_4^2 + 180s_4s_2^2 + 160s_3^2s_2 - 15s_2^4)/M^{[7]}$$

$$+ 180(-120s_8 + 84s_6s_2 + 64s_5s_3 + 30s_4^2 - 33s_4s_2^2 - 28s_3^2s_2 + 3s_2^4)/M^{[6]}$$

$$- 72(24s_8 - 20s_6s_2 - 12s_5s_3 - 6s_4^2 + 9s_4s_2^2 + 6s_3^2s_2 - s_2^4)/M^{[5]}$$

$$+ 9(-6s_8 + 8s_6s_2 + 3s_4^2 - 6s_4s_2^2 + s_2^4)/M^{[4]}$$

$$+ 48(-120s_8 + 60s_6s_2 + 64s_5s_3 + 30s_4^2 - 15s_4s_2^2 - 20s_3^2s_2)/M^{[6]}$$

$$- 96(24s_8 - 12s_6s_2 - 14s_5s_3 - 6s_4^2 + 3s_4s_2^2 + 5s_3^2s_2)/M^{[5]}$$

$$+ 24(-6s_6 + 4s_6s_2 + 4s_5s_3 + s_4^2 - s_4s_2^2 - 2s_3^2s_2)/M^{[4]}$$

$$+ 16(-6s_8 + s_6s_2 + 4s_5s_3 + 2s_4^2 - s_3^2s_2)/M^{[4]}$$

$$- 12(24s_8 - 12s_6s_2 - 8s_5s_3 - 6s_4^2 + 3s_4s_2^2)/M^{[5]}$$

$$+ 24(-6s_8 + 3s_6s_2 + 2s_5s_3 + 2s_4^2 - s_4s_2^2)/M^{[4]}$$

$$- 6(2s_8 - 2s_6s_2 - s_4^2 + s_4s_2^2)/M^{[3]}$$

$$- 8(2s_8 - s_5s_3 - s_4^2)/M^{[3]}$$

$$+ (-s_8 + s_4^2)/M^{[2]}$$

$$= (-181440s_8 + 120960s_6s_2 + 96768s_5s_3 + 45360s_4^2 - 45360s_4s_2^2 - 40320s_3^2s_2 + 3780s_2^4)/M^{[8]}$$

$$+ (-103680s_8 + 69120s_6s_2 + 55296s_5s_3 + 25920s_4^2 - 25920s_4s_2^2 - 23040s_3^2s_2 + 2160s_2^4)/M^{[7]}$$

$$+ (-21600s_8 + 15120s_6s_2 + 11520s_5s_3 + 5400s_4^2 - 5940s_4s_2^2 - 5040s_3^2s_2$$
$$+ 540s_2^4 - 5760s_8 + 2880s_6s_2 + 3072s_5s_3 + 1440s_4^2 - 720s_4s_2^2$$
$$- 960s_3^2s_2)/M^{[6]}$$
$$+ (-1728s_8 + 1440s_6s_2 + 864s_5s_3 + 432s_4^2 - 648s_4s_2^2 - 432s_3^2s_2$$
$$+ 72s_2^4 - 2304s_8 + 1152s_6s_2 + 1344s_5s_3 + 576s_4^2 - 288s_4s_2^2$$
$$- 480s_3^2s_2 - 288s_8 + 144s_6s_2 + 96s_5s_3 + 72s_4^2 - 36s_4s_2^2)/M^{[5]}$$
$$+ (-54s_8 + 72s_6s_2 + 27s_4^2 - 54s_4s_2^2 + 9s_2^4 - 144s_8 + 96s_6s_2 + 96s_5s_3$$
$$+ 24s_4^2 - 24s_4s_2^2 - 48s_3^2s_2 - 96s_8 + 16s_6s_2 + 64s_5s_3 + 32s_4^2$$
$$- 16s_3^2s_2 - 144s_8 + 72s_6s_2 + 48s_5s_3 + 48s_4^2 - 24s_4s_2^2)/M^{[4]}$$
$$+ (-12s_8 + 12s_6s_2 + 6s_4^2 - 6s_4s_2^2 - 16s_8 + 8s_5s_3 + 8s_4^2)/M^{[3]}$$
$$+ (-s_8 + s_4^2)/M^{[2]}$$
$$= (-181440s_8 + 120960s_6s_2 + 96768s_5s_3 + 45360s_4^2 - 45360s_4s_2^2$$
$$- 40320s_3^2s_2 + 3780s_2^4)/M^{[8]}$$
$$+ (-103680s_8 + 69120s_6s_2 + 55296s_5s_3 + 25920s_4^2 - 25920s_4s_2^2$$
$$- 23040s_3^2s_2 + 2160s_2^4)/M^{[7]}$$
$$+ (-27360s_8 + 18000s_6s_2 + 14592s_5s_3 + 6840s_4^2 - 6660s_4s_2^2$$
$$- 6000s_3^2s_2 + 540s_2^4)/M^{[6]}$$
$$+ (-4320s_8 + 2736s_6s_2 + 2304s_5s_3 + 1080s_4^2 - 972s_4s_2^2$$
$$-912s_3^2s_2 + 72s_2^4)/M^{[5]}$$
$$+ (-438s_8 + 256s_6s_2 + 208s_5s_3 + 131s_4^2 - 102s_4s_2^2 - 64s_3^2s_2$$
$$+ 9s_2^4)/M^{[4]}$$

$$+ (-28s_8 + 12s_6s_2 + 8s_5s_3 + 14s_4^2 - 6s_4s_2^2)/M^{[3]}$$

$$+ (-s_8 + s_4^2)/M^{[2]}$$

$$= m_8M(- \frac{1}{M^{[2]}} - \frac{28}{M^{[3]}} - \frac{438}{M^{[4]}} - \frac{4320}{M^{[5]}} - \frac{27360}{M^{[6]}} - \frac{103680}{M^{[7]}} - \frac{181440}{M^{[8]}})$$

$$+ m_6m_2M^2(\frac{12}{M^{[3]}} + \frac{256}{M^{[4]}} + \frac{2736}{M^{[5]}} + \frac{18000}{M^{[6]}} + \frac{69120}{M^{[7]}} + \frac{120960}{M^{[8]}})$$

$$+ m_5m_3M^2(\frac{8}{M^{[3]}} + \frac{208}{M^{[4]}} + \frac{2304}{M^{[5]}} + \frac{14592}{M^{[6]}} + \frac{55296}{M^{[7]}} + \frac{96768}{M^{[8]}})$$

$$+ m_4^2M^2(\frac{1}{M^{[2]}} + \frac{14}{M^{[3]}} + \frac{131}{M^{[4]}} + \frac{1080}{M^{[5]}} + \frac{6840}{M^{[6]}} + \frac{25920}{M^{[7]}} + \frac{45360}{M^{[8]}})$$

$$+ m_4m_2^2M^3(- \frac{6}{M^{[3]}} - \frac{102}{M^{[4]}} - \frac{972}{M^{[5]}} - \frac{6660}{M^{[6]}} - \frac{25920}{M^{[7]}} - \frac{45360}{M^{[8]}})$$

$$+ m_3^2m_2M^3(- \frac{64}{M^{[4]}} - \frac{912}{M^{[5]}} - \frac{6000}{M^{[6]}} - \frac{23040}{M^{[7]}} - \frac{40320}{M^{[8]}})$$

$$+ m_2^4M^4(\frac{9}{M^{[4]}} + \frac{72}{M^{[5]}} + \frac{540}{M^{[6]}} + \frac{2160}{M^{[7]}} + \frac{3780}{M^{[8]}}) . \qquad \text{(C34)}$$

This completes the present task. Expressions for the terms k_{22}, k_{42}, and k_{44} appearing in the estimates of the variance for the jump rate are now available in terms of sample moments, allowing an immediate estimate of the errors from the experimental results themselves.

APPENDIX D

COMPUTER PROGRAMS AND TABLES

```
C       PPLOT
C
C       THE PURPOSE OF THE PROGRAM PPLOT IS TO CALCULATE AND PLOT
C       THE PROBABILITY THAT AN ADATOM STARTING AT THE ORIGIN HOPS
C       TO A POSITION "I" LATTICE SPACINGS TO THE RIGHT.  THIS
C       PROBABILITY IS ASSESSED FOR VARIOUS VALUES OF THE JUMP
C       RATE RATIO B/A AND THE SECOND MOMENT M2.
C
        IMPLICIT REAL(M)
        DIMENSION BOA(5),FUNC(25,5)
        DIMENSION RIA(50),RIB(50),BESIA(50),BESIB(50)
        COMMON FUNC
    5   TYPE 95
        ACCEPT 100,N
        IF (N.EQ.0) STOP
C
C       SET THE NUMBER OF TERMS "N" EQUAL TO ZERO IN ORDER TO
C       TERMINATE EXECUTION OF PPLOT.
C
        ACCEPT 110,BOA(1)
        ACCEPT 110,BOA(2)
        ACCEPT 110,BOA(3)
        TYPE 140
        ACCEPT 110,M2
        TYPE 115
        DO 50 J=1,3
        DO 50 NSTEP=0,24
        A=M2/(2.+8.*BOA(J))
        B=BOA(J)*A
        CALL IC(2.*A,RICA)
        CALL IC(2.*B,RICB)
        CALL INUE(2.*A,N,RICA,RIA)
        CALL INUE(2.*B,N,RICB,RIB)
        NP4=N+4
        NT2=2*N
        DO 10 I=1,N
        BESIA(NP4-I)=RIA(I)
        BESIA(I+NP4)=RIA(I)
        BESIB(NP4-I)=RIB(I)
   10   BESIB(I+NP4)=RIB(I)
        BESIA(NP4)=RICA
        BESIB(NP4)=RICB
        NODD=2*(N/2)+1
        NEVN=2*(N/2)
        ISTRT2=(2-NEVN)/2
        ISTOP2=(2+NEVN)/2
        ISTRT1=(1-NODD)/2
        ISTOP1=(1+NODD)/2
        DBLP2=0.
        DO 20 K=ISTRT2,ISTOP2
        DBLP2=DBLP2+EXP(-2.*B)*BESIB(K+NP4)
       1*EXP(-2.*A)*BESIA(NSTEP-2*K+NP4)
   20   CONTINUE
        FUNC(NSTEP,J)=DBLP2
   50   CONTINUE
        DO 60 I=0,6
   60   TYPE 130,I,FUNC(I,1),FUNC(I,2),FUNC(I,3)
   95   FORMAT(' GIVE THE # OF TERMS, AND THE 3 VALUES FOR B/A')
  100   FORMAT(I2)
  110   FORMAT(G12.6)
  115   FORMAT(2H1 )
```

```
130   FORMAT(1H ,I2,5H     ,3(E12.6,2H  ))
140   FORMAT(' GIVE THE VALUE OF THE SECOND MOMENT')
160   FORMAT(1H ,G12.6)
      CALL PLOT
      GO TO 5
      END
C
C     THE SUBROUTINE "IC" CALCULATES A ZEROTH ORDER MODIFIED
C     BESSEL FUNCTION FOR A GIVEN ARGUMENT "X" AND ASSIGNS THE
C     VALUE OF THE FUNCTION TO "RIC".
C
      SUBROUTINE IC(X,RIC)
      RIC=ABS(X)
      IF(RIC-3.75)1,1,2
    1 Z=X*X*7.111111E-2
      RIC=(((((4.5813E-3*Z+3.60768E-2)*Z+2.659732E-1)*Z+1.206749E0)*Z
     1+3.089942E0)*Z+3.515623E0)*Z+1.
      RETURN
    2 Z=3.75/RIC
      RIC= EXP(RIC)/SQRT(RIC)*((((((((3.92377E-3*Z-1.647633E-2)*Z
     1+2.635537E-2)*Z-2.057706E-2)*Z+5.16281E-3)*Z-1.57565E-3)*Z
     2+2.25319E-3)*Z+1.328592E-2)*Z+3.989423E-1)
      RETURN
      END
C
C     THE SUBROUTINE "INUE" CALCULATES A SET OF MODIFIED BESSEL
C     FUNCTIONS OF ORDERS 1 THROUGH "N" FOR A GIVEN ARGUMENT
C     "X" AND THE VALUE OF THE CORRESPONDING ZEROTH ORDER BESSEL
C     FUNCTION "ZI".  THE VALUES OF THE BESSEL FUNCTIONS FOR
C     ORDERS 1 THROUGH "N" ARE ASSIGNED TO THE ONE DIMENSIONAL
C     ARRAY "RI".
C
      SUBROUTINE INUE(X,N,ZI,RI)
      DIMENSION RI(50)
      IF (N)10,10,1
    1 FN=N+N
      Q1=X/FN
      IF (ABS(X)-5.E-4)6,6,2
    2 A0=1.
      A1=0.
      B0=0.
      B1=1.
      FI =FN
    3 FI=FI+2
      AN=FI/ABS(X)
      A=AN*A1+A0
      B=AN*B1+B0
      A0=A1
      B0=B1
      A1=A
      B1=B
      Q0=Q1
      Q1=A/B
      IF (ABS((Q1-Q0)/Q1)-1.E-6)4,4,3
    4 IF(X)5,6,6
    5 C1=-Q1
    6 K=N
    7 Q1=X/(FN+X*Q1)
      RI(K)=Q1
      FN=FN-2
      K=K-1
```

```
      IF(K)8,8,7
    8 FI=ZI
      DO 9 I=1,N
      FI=FI*RI(I)
    9 RI(I)=FI
   10 RETURN
      END
C
C     THE SUBROUTINE "PLOT" PLOTS THE PROBABILITY IN QUESTION
C     AS A FUNCTION OF LATTICE POSITION.
C
      SUBROUTINE PLOT
      REAL LINE
      DIMENSION LINE(90),FUNC(25,5),ALPHA(10)
      COMMON FUNC
      TYPE 170
      ACCEPT 180,SCALE
      TYPE 160
      ACCEPT 120,(ALPHA(I),I=1,5)
      TYPE 150
      DO 30 I=1,77
   30 LINE(I)=ALPHA(4)
      TYPE 110,(LINE(I),I=1,77)
      DO 50 I=0,6
      DO 35 K=2,76
35    LINE(K)=ALPHA(5)
      DO 40 J=1,3
      IFUNC=FUNC(I,J)*72./SCALE+.5
40    LINE(IFUNC+2)=ALPHA(J)
50    TYPE 130,I,(LINE(K),K=1,77)
100   FORMAT(1H1,A77)
110   FORMAT(1H ,77A1)
120   FORMAT(6A1)
130   FORMAT(1H ,I2,77A1)
150   FORMAT(2H1 )
160   FORMAT(' GIVE THE FIVE ALPHANUMERIC VALUES (E.G. 123. ):')
170   FORMAT(' WHAT IS THE SCALE?')
180   FORMAT(G12.6)
      END
```

```
C       KPLOT
C
C       THIS PROGRAM "KPLOT" IS DESIGNED TO CALCULATE THE VALUES FOR THE
C       STANDARD DEVIATIONS OF ALPHA-T AND BETA-T.  THE FOLLOWING SYMBOLS
C       WILL BE USED THROUGHOUT THE PROGRAM, AND WILL BE GIVEN THE
C       ADJACENT DEFINITIONS:
C       ALPT...THE PRODUCT OF "ALPHA" AND "T".
C       BTAT...THE PRODUCT OF "BETA" AND "T".
C       M2  ...THE 2ND PARENT MOMENT.
C       ERRA...THE STANDARD DEVIATION OF ALPT DIVIDED BY ALPT.
C       ERRB...THE STANDARD DEVIATION OF BTAT DIVIDED BY BTAT.
C       INDX...A LABEL FOR THE 24 VALUES OF M2.
C
C       NOTE, THAT FOR THIS PROGRAM, THE DISTANCE BETWEEN ADJACENT SITES
C       IS ASSUMED TO BE UNITY.
C
        IMPLICIT REAL(K,M,N)
        DIMENSION FUNC(25,5),AP(6)
        COMMON FUNC
        ITABLE=0
   10   TYPE 180
        ACCEPT 150,M
        IF (M.LT.1.) STOP
        IM=M
        ITABLE=ITABLE+1
        TYPE 140
        TYPE 170,ITABLE,M
        TYPE 130
        TYPE 130
        TYPE 160
        DO 50 J=1,2
        TYPE 130
        DO 50 C=1.,24.
        RJ=J
        I=C+1.
        X=C/8.-2.
        M2=10.**X
C
C       A IS EQUIVALENT TO ALPHA-T; B IS EQUIVALENT TO BETA-T.
C       M2 IS EQUIVALENT TO THE MEAN SQUARE DISPLACEMENT OF THE
C       DIFFUSING ADATOM.
C
        A=M2/(2.+.8*RJ)
        B=RJ*A/10.
        I0=2*J-1
        I1=2*J
C
C       THIS PART OF THE PROGRAM CALCULATES ERRA & ERRB.
C
        N8=512.*B+2.*A+64512.*B**2+252.*A**2+12096.*A*B+20160.*B
       1*(4*B+A)**2+1680.*(4*B+A)**3+1680.*(4*B+A)**4
        N6=128.*B+2.*A+60.*(4.*B+A)**2+720.*B*(4.*B+A)+120.
       1*(4.*B+A)**3
        N4=2.*A+32.*B+12.*(4*B+A)**2
        N2=2.*(4.*B+A)
        K8=N8-28.*N6*N2-35.*N4**2+420.*N4*N2**2-630.*N2**4
        K6=N6-15.*N4*N2+30.*N2**3
        K4=N4-3.*N2**2
        K2=N2
        VA=(K8/M+16.*K6*K2/(M-1.)+(M+33.)*K4**2/(M-1.)
       1+72.*M*K4*K2**2/(M-1.))/(M-2.)
```

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```
     1+24.*M*(M+1.)*K2**4/(M-1.)/(M-2.)/(M-3.)
     1-8.*K6/M-8.*(M+7.)*K4*K2/(M-1.)
     1+16.*K4/M+16.*(M+1.)*K2**2/(M-1.))/36.-A**2.
      VB=(K8/M+16.*K6*K2/(M-1.)+(M+33.)*K4**2/(M-1.)
     1+72.*M*K4*K2**2/(M-1.)/(M-2.)
     1+24.*M*(M+1.)*K2**4/(M-1.)/(M-2.)/(M-3.)
     1-2.*K6/M-2.*(M+7.)*K4*K2/(M-1.)
     1+K4/M+(M+1.)*K2**2/(M-1.))/576.-B**2
      STA=VA**.5/A
      STB=VB**.5/B
      FUNC(I,I0)=ALOG10(STA)
      FUNC(I,I1)=ALOG10(STB)
C
C     THIS STATEMENT CREATES THE TABLE ENTREES.
C
      IC=C
 30   TYPE 110,A,B,M2,STA,STB,IC
 50   CONTINUE
 100  FORMAT(1H ,6(4H    ,A4,4H    ))
 110  FORMAT(1H ,5E12.6,I6)
 120  FORMAT(A4)
 130  FORMAT(2H  )
 140  FORMAT(2H1 )
 150  FORMAT(G12.2)
 160  FORMAT(1H ,4X,'ALPT',8X,'BTAT',8X,'M2',10X,'ERRA',8X,
     1'ERRB',8X,'INDX')
 170  FORMAT(1H ,'TABLE N',I1,5X,'M= ',E9.2)
 180  FORMAT(1H ,'WHAT IS THE NUMBER OF OBSERVATIONS?')


C
C     THIS SUBROUTINE PLOTS ERRA AND ERRB AS FUNCTIONS OF M2 ON A
C     THREE TIERED LOG-LOG SCALE.  THE KEY BELOW INDICATES
C     WHICH SYMBOLS CORRESPOND TO WHICH VALUES:
C
C     1...ERRA WHEN B=A/10
C     2...ERRB WHEN B=A/10
C     3...ERRA WHEN B=A/5
C     4...ERRB WHEN B=A/5
C
      CALL PLOT
      GO TO 10
      END
C
      SUBROUTINE PLOT
      REAL LINE
      DIMENSION LINE(90),FUNC(25,5),ALPHA(10)
      COMMON FUNC
      TYPE 160
      ACCEPT 120,(ALPHA(I),I=1,6)
      TYPE 150
      DO 30 I=1,77
 30   LINE(I)=ALPHA(5)
      TYPE 110,(LINE(I),I=1,77)
      DO 50 I=1,24
      DO 35 K=2,76
 35   LINE(K)=ALPHA(6)
      DO 40 J=1,4
      IFUNC=FUNC(I,J)*25+49.5
 40   LINE(IFUNC+2)=ALPHA(J)
      IM1=I-1
```

```
50   TYPE 130,IM1,(LINE(K),K=1,77)
100  FORMAT(1H1,A77)
110  FORMAT(1H ,77A1)
120  FORMAT(6A1)
130  FORMAT(1H ,1I2,77A1)
150  FORMAT(1H1)
160  FORMAT(1H ,'WRITE 1234. AND A BLANK')
     END
```

```
C       MPLOT
C
C       THIS PROGRAM "MPLOT" IS DESIGNED TO CALCULATE THE VALUES FOR THE
C       STANDARD DEVIATIONS OF ALPHA-T AND BETA-T.  THE FOLLOWING SYMBOLS
C       WILL BE USED THROUGHOUT THE PROGRAM, AND WILL BE GIVEN THE
C       ADJACENT DEFINITIONS:
C       ERRA...THE STANDARD DEVIATION OF ALPT DIVIDED BY ALPT.
C       ERRB...THE STANDARD DEVIATION OF BTAT DIVIDED BY BTAT.
C       INDX...A LABEL FOR THE 24 VALUES OF THE SECOND MOMENT M2.
C
C       NOTE, THAT FOR THIS PROGRAM, THE DISTANCE BETWEEN ADJACENT SITES
C       IS ASSUMED TO BE UNITY.
C
        IMPLICIT REAL (K,M,N)
        DIMENSION FUNC(25,9),AP(6)
        COMMON FUNC
 10     TYPE 180
        ACCEPT 150,M2
        DO 50 J=1,2
        TYPE 130
        RJ=J
        DO 50 I=1,25
        M=500*I
C
C       A IS EQUIVALENT TO ALPHA-T; B IS EQUIVALENT TO BETA-T.
C       M2 IS EQUIVALENT TO THE MEAN SQUARE DISPLACEMENT OF THE
C       DIFFUSING ADATOM.
C
        A=M2/(2.+.8*RJ)
        B=RJ*A/10.
        I0=2*J-1
        I1=2*J
C
C       THIS PART OF THE PROGRAM CALCULATES ERRA & ERRB.
C
        N8=512.*B+2.*A+64512.*B**2+252.*A**2+12096.*A*B+20160.*B
       1*(4*B+A)**2+1752.*(4*B+A)**3+1680.*(4*B+A)**4
        N6=128.*B+2.*A+60.*(4.*B+A)**2+720.*B*(4.*B+A)+120.
       1*(4.*B+A)**3
        N4=2.*A+32.*B+12.*(4*B+A)**2
        N2=2.*(4.*B+A)
        K8=N8-28.*N6*N2-35.*N4**2+420.*N4*N2**2-630.*N2**4
        K6=N6-15.*N4*N2+30.*N2**3
        K4=N4-3.*N2**2
        K2=N2
        VA=(K8/M+16.*K6*K2/(M-1.)+(M+33.)*K4**2/(M-1.)
       1+72.*M*K4*K2**2/(M-1.)/(M-2.)
       1+24.*M*(M+1.)*K2**4/(M-1.)/(M-2.)/(M-3.)
       1-8.*K6/M-8.*(M+7.)*K4*K2/(M-1.)
       1+16.*K4/M+16.*(M+1.)*K2**2/(M-1.))/36.-A**2.
        VB=(K8/M+16.*K6*K2/(M-1.)+(M+33.)*K4**2/(M-1.)
       1+72.*M*K4*K2**2/(M-1.)/(M-2.)
       1+24.*M*(M+1.)*K2**4/(M-1.)/(M-2.)/(M-3.)
       1-2.*K6/M-2.*(M+7.)*K4*K2/(M-1.)
       1+K4/M+(M+1.)*K2**2/(M-1.))/576.-B**2
        STA=VA**.5/A
        STB=VB**.5/B
        FUNC(I,I0)=STA
        FUNC(I,I1)=STB
 50     CONTINUE
 100    FORMAT(1H ,6(4H    ,A4,4H    ))
```

```
110   FORMAT(1H ,5E12.6,I6)
120   FORMAT(A4)
130   FORMAT(2H )
140   FORMAT(2H1 )
150   FORMAT(G12.6)
180   FORMAT(1H ,'WHAT IS THE SECOND MOMENT?')
C
C     THE SUBROUTINE "PLOT" PLOTS ERRA AND ERRB AS  FUNCTIONS OF THE
C     NUMBER OF DIFFUSION INTERVALS "M".  THE KEY BELOW INDICATES
C     WHICH SYMBOLS CORRESPOND TO WHICH VALUES.
C
C     1...ERRA WHEN B=A/10
C     2...ERRB WHEN B=A/10
C     3...ERRA WHEN B=A/5
C     4...ERRB WHEN B=A/5
C
      CALL PLOT
      END
      SUBROUTINE PLOT
      REAL LINE
      DIMENSION LINE(90),FUNC(25,5),ALPHA(10)
      COMMON FUNC
      TYPE 160
      ACCEPT 120,(ALPHA(I),I=1,6)
      TYPE 150
      DO 30 I=1,77
30    LINE(I)=ALPHA(5)
      TYPE 110,(LINE(I),I=1,77)
      DO 50 I=1,24
      DO 35 K=2,76
35    LINE(K)=ALPHA(6)
      DO 40 J=1,4
      IFUNC=FUNC(I,J)*70.+.5
40    LINE(IFUNC+2)=ALPHA(J)
      IM1=I-1
50    TYPE 130,IM1,(LINE(K),K=1,77)
100   FORMAT(1H1,A77)
110   FORMAT(1H ,77A1)
120   FORMAT(6A1)
130   FORMAT(1H ,1I2,77A1)
150   FORMAT(1H1)
160   FORMAT(1H ,'WRITE 1234, AND A BLANK')
      END
```

TABLE D1 M= 0.10E+03

ALPT	BTAT	M2	ERRA	ERRB	INDX
.476258E-02	.476258E-03	.133352E-01	.114315E+01	.359410E+01	1
.635100E-02	.635100E-03	.177828E-01	.102253E+01	.320939E+01	2
.846919E-02	.846919E-03	.237137E-01	.922200E+00	.288832E+01	3
.112938E-01	.112938E-02	.316228E-01	.839759E+00	.262313E+01	4
.150606E-01	.150606E-02	.421697E-01	.773097E+00	.240699E+01	5
.200836E-01	.200836E-02	.562341E-01	.720378E+00	.223386E+01	6
.267819E-01	.267819E-02	.749894E-01	.680033E+00	.209845E+01	7
.357143E-01	.357143E-02	.100000E+00	.650772E+00	.199626E+01	8
.476258E-01	.476258E-02	.133352E+00	.631614E+00	.192359E+01	9
.635100E-01	.635100E-02	.177828E+00	.621936E+00	.187774E+01	10
.846919E-01	.846919E-02	.237137E+00	.621528E+00	.185711E+01	11
.112938E+00	.112938E-01	.316228E+00	.630654E+00	.186143E+01	12
.150606E+00	.150606E-01	.421697E+00	.650133E+00	.189191E+01	13
.200836E+00	.200836E-01	.562341E+00	.681430E+00	.195158E+01	14
.267819E+00	.267819E-01	.749894E+00	.726787E+00	.204561E+01	15
.357143E+00	.357143E-01	.100000E+01	.789409E+00	.218184E+01	16
.476258E+00	.476258E-01	.133352E+01	.873743E+00	.237148E+01	17
.635100E+00	.635100E-01	.177828E+01	.985863E+00	.263006E+01	18
.846919E+00	.846919E-01	.237137E+01	.113403E+01	.297875E+01	19
.112938E+01	.112938E+00	.316228E+01	.132945E+01	.344618E+01	20
.150606E+01	.150606E+00	.421696E+01	.158728E+01	.407089E+01	21
.200836E+01	.200836E+00	.562341E+01	.192798E+01	.490452E+01	22
.267819E+01	.267819E+00	.749894E+01	.237906E+01	.601620E+01	23
.357143E+01	.357143E+00	.100000E+02	.297744E+01	.749836E+01	24
.370423E-02	.740845E-03	.133352E-01	.143201E+01	.288271E+01	1
.493967E-02	.987933E-03	.177828E-01	.130991E+01	.257418E+01	2
.658715E-02	.131743E-02	.237137E-01	.121096E+01	.231656E+01	3
.878410E-02	.175682E-02	.316228E-01	.113205E+01	.210356E+01	4
.117138E-01	.234276E-02	.421697E-01	.107043E+01	.192965E+01	5
.156206E-01	.312412E-02	.562341E-01	.102370E+01	.178988E+01	6
.208304E-01	.416608E-02	.749894E-01	.989862E+00	.167988E+01	7
.277778E-01	.555556E-02	.100000E+00	.967362E+00	.159588E+01	8
.370423E-01	.740845E-02	.133352E+00	.955135E+00	.153471E+01	9
.493967E-01	.987933E-02	.177828E+00	.952645E+00	.149395E+01	10
.658715E-01	.131743E-01	.237137E+00	.959933E+00	.147195E+01	11
.878410E-01	.175682E-01	.316228E+00	.977675E+00	.146802E+01	12
.117138E+00	.234276E-01	.421697E+00	.100726E+01	.148254E+01	13
.156206E+00	.312412E-01	.562341E+00	.105091E+01	.151709E+01	14
.208304E+00	.416608E-01	.749894E+00	.111182E+01	.157477E+01	15
.277778E+00	.555556E-01	.100000E+01	.119442E+01	.166039E+01	16
.370423E+00	.740845E-01	.133352E+01	.130468E+01	.178101E+01	17
.493966E+00	.987933E-01	.177828E+01	.145066E+01	.194650E+01	18
.658715E+00	.131743E+00	.237137E+01	.164311E+01	.217036E+01	19
.878410E+00	.175682E+00	.316228E+01	.189651E+01	.247092E+01	20
.117138E+01	.234276E+00	.421696E+01	.223035E+01	.287284E+01	21
.156206E+01	.312412E+00	.562341E+01	.267086E+01	.340925E+01	22
.208304E+01	.416608E+00	.749894E+01	.325330E+01	.412451E+01	23
.277778E+01	.555556E+00	.100000E+02	.402501E+01	.507796E+01	24

TABLE 02 M= 0.10E+04

ALPT	BTAT	M2	ERRA	ERRB	INDX
.476258E-02	.476258E-03	.133352E-01	.361166E+00	.113557E+01	1
.635100E-02	.635100E-03	.177829E-01	.322977E+00	.101379E+01	2
.846919E-02	.846919E-03	.237137E-01	.291201E+00	.912118E+00	3
.112938E-01	.112938E-02	.316228E-01	.265077E+00	.828107E+00	4
.150606E-01	.150606E-02	.421697E-01	.243937E+00	.759596E+00	5
.200836E-01	.200836E-02	.562341E-01	.227201E+00	.704674E+00	6
.267819E-01	.267819E-02	.749894E-01	.214369E+00	.661568E+00	7
.357143E-01	.357143E-02	.100000E+00	.205033E+00	.629143E+00	8
.476258E-01	.476258E-02	.133352E+00	.198877E+00	.605929E+00	9
.635100E-01	.635100E-02	.177828E+00	.195699E+00	.591158E+00	10
.846919E-01	.846919E-02	.237137E+00	.195425E+00	.584306E+00	11
.112938E+00	.112938E-01	.316228E+00	.198125E+00	.585257E+00	12
.150606E+00	.150606E-01	.421697E+00	.204053E+00	.594362E+00	13
.200836E+00	.200836E-01	.562341E+00	.213644E+00	.612527E+00	14
.267819E+00	.267819E-01	.749894E+00	.227584E+00	.641324E+00	15
.357143E+00	.357143E-01	.100000E+01	.246852E+00	.683140E+00	16
.476258E+00	.476258E-01	.133352E+01	.272807E+00	.741394E+00	17
.635100E+00	.635100E-01	.177828E+01	.307304E+00	.820827E+00	18
.846919E+00	.846919E-01	.237137E+01	.352968E+00	.927911E+00	19
.112938E+01	.112938E+00	.316228E+01	.412922E+00	.107140E+01	20
.150606E+01	.150606E+00	.421696E+01	.492100E+00	.126307E+01	21
.200836E+01	.200836E+00	.562341E+01	.596661E+00	.151873E+01	22
.267819E+01	.267819E+00	.749894E+01	.735024E+00	.185955E+01	23
.357143E+01	.357143E+00	.100000E+02	.918489E+00	.231382E+01	24
.370423E-02	.740845E-03	.133352E-01	.452128E+00	.910810E+00	1
.493967E-02	.987933E-03	.177828E-01	.413439E+00	.813142E+00	2
.658715E-02	.131743E-02	.237137E-01	.382070E+00	.731564E+00	3
.878410E-02	.175682E-02	.316228E-01	.357039E+00	.664093E+00	4
.117138E-01	.234276E-02	.421697E-01	.337471E+00	.608973E+00	5
.156206E-01	.312412E-02	.562341E-01	.322609E+00	.564643E+00	6
.208304E-01	.416608E-02	.749894E-01	.311817E+00	.529721E+00	7
.277778E-01	.555556E-02	.100000E+00	.304601E+00	.503009E+00	8
.370423E-01	.740845E-02	.133352E+00	.300617E+00	.483503E+00	9
.493967E-01	.987933E-02	.177828E+00	.299689E+00	.470425E+00	10
.658715E-01	.131743E-01	.237137E+00	.301817E+00	.463247E+00	11
.878410E-01	.175682E-01	.316228E+00	.307203E+00	.461732E+00	12
.117138E+00	.234276E-01	.421697E+00	.316268E+00	.465976E+00	13
.156206E+00	.312412E-01	.562341E+00	.329687E+00	.476454E+00	14
.208304E+00	.416608E-01	.749894E+00	.348442E+00	.494093E+00	15
.277778E+00	.555556E-01	.100000E+01	.373887E+00	.520368E+00	16
.370423E+00	.740845E-01	.133352E+01	.407854E+00	.557427E+00	17
.493966E+00	.987933E-01	.177828E+01	.452801E+00	.608283E+00	18
.658715E+00	.131743E+00	.237137E+01	.512023E+00	.677065E+00	19
.878410E+00	.175682E+00	.316228E+01	.589945E+00	.769372E+00	20
.117138E+01	.234276E+00	.421696E+01	.692523E+00	.892745E+00	21
.156206E+01	.312412E+00	.562341E+01	.827779E+00	.105732E+01	22
.208304E+01	.416608E+00	.749894E+01	.100650E+01	.127667E+01	23
.277778E+01	.555556E+00	.100000E+02	.124318E+01	.156896E+01	24

TABLE D3 M= 0.10E+05

ALPT	BTAI	M2	ERRA	ERRB	INDX
.476258E-02	.476258E-03	.133352E-01	.114200E+00	.359069E+00	1
.635100E-02	.635100E-03	.177828E-01	.102122E+00	.320554E+00	2
.846919E-02	.846919E-03	.237137E-01	.920729E-01	.288398E+00	3
.112938E-01	.112938E-02	.316228E-01	.838094E-01	.261827E+00	4
.150606E-01	.150606E-02	.421697E-01	.771229E-01	.240157E+00	5
.200836E-01	.200836E-02	.562341E-01	.718281E-01	.222783E+00	6
.267819E-01	.267819E-02	.749894E-01	.677684E-01	.209177E+00	7
.357143E-01	.357143E-02	.100000E+00	.648135E-01	.198886E+00	8
.476258E-01	.476258E-02	.133352E+00	.628639E-01	.191538E+00	9
.635100E-01	.635100E-02	.177828E+00	.618554E-01	.186858E+00	10
.846919E-01	.846919E-02	.237137E+00	.617635E-01	.184681E+00	11
.112938E+00	.112938E-01	.316228E+00	.626135E-01	.184969E+00	12
.150606E+00	.150606E-01	.421697E+00	.644795E-01	.187832E+00	13
.200836E+00	.200836E-01	.562341E+00	.675027E-01	.193554E+00	14
.267819E+00	.267819E-01	.749894E+00	.718985E-01	.202632E+00	15
.357143E+00	.357143E-01	.100000E+01	.779753E-01	.215816E+00	16
.476258E+00	.476258E-01	.133352E+01	.861608E-01	.234185E+00	17
.635100E+00	.635100E-01	.177828E+01	.970403E-01	.259233E+00	18
.846919E+00	.846919E-01	.237137E+01	.111410E+00	.292997E+00	19
.112938E+01	.112938E+00	.316228E+01	.130346E+00	.338239E+00	20
.150606E+01	.150606E+00	.421696E+01	.155312E+00	.398669E+00	21
.200836E+01	.200836E+00	.562341E+01	.188280E+00	.479272E+00	22
.267819E+01	.267819E+00	.749894E+01	.231902E+00	.586718E+00	23
.357143E+01	.357143E+00	.100000E+02	.289741E+00	.729926E+00	24
.370423E-02	.740845E-03	.133352E-01	.142953E+00	.287999E+00	1
.493967E-02	.987933E-03	.177828E-01	.130716E+00	.257110E+00	2
.658715E-02	.131743E-02	.237137E-01	.120794E+00	.231310E+00	3
.878410E-02	.175682E-02	.316228E-01	.112876E+00	.209970E+00	4
.117138E-01	.234276E-02	.421697E-01	.106686E+00	.192536E+00	5
.156206E-01	.312412E-02	.562341E-01	.101983E+00	.178513E+00	6
.208304E-01	.416608E-02	.749894E-01	.985673E-01	.167465E+00	7
.277778E-01	.555556E-02	.100000E+00	.962829E-01	.159014E+00	8
.370423E-01	.740845E-02	.133352E+00	.950192E-01	.152840E+00	9
.493967E-01	.987933E-02	.177828E+00	.947210E-01	.148699E+00	10
.658715E-01	.131743E-01	.237137E+00	.953883E-01	.146422E+00	11
.878410E-01	.175682E-01	.316228E+00	.970855E-01	.145935E+00	12
.117138E+00	.234276E-01	.421697E+00	.999420E-01	.147266E+00	13
.156206E+00	.312412E-01	.562341E+00	.104174E+00	.150565E+00	14
.208304E+00	.416608E-01	.749894E+00	.110090E+00	.156125E+00	15
.277778E+00	.555556E-01	.100000E+01	.118115E+00	.164409E+00	16
.370423E+00	.740845E-01	.133352E+01	.128828E+00	.176095E+00	17
.493966E+00	.987933E-01	.177828E+01	.143005E+00	.192132E+00	18
.658715E+00	.131743E+00	.237137E+01	.161682E+00	.213821E+00	19
.878410E+00	.175682E+00	.316228E+01	.186255E+00	.242926E+00	20
.117138E+01	.234276E+00	.421696E+01	.218601E+00	.281826E+00	21
.156206E+01	.312412E+00	.562341E+01	.261248E+00	.333713E+00	22
.208304E+01	.416608F+00	.749894E+01	.317597E+00	.402868E+00	23
.277778E+01	.555556E+00	.100000E+02	.392216E+00	.495014E+00	24

APPENDIX E

TABLES OF POWER SUMS AND k-STATISTICS IN TERMS OF AUGMENTED SYMMETRIC FUNCTIONS

In Algorithm B1 of Appendix B, we outlined a procedure for finding the unbiased estimator of a given population value. We found that this estimate could often be simply expressed in terms of k-statistics. In order to generate a given k-statistic from a data set however, it is best expressed in terms of sample moments about the mean. By expressing a k-statistic in terms of augmented symmetric functions and then finding these augmented symmetric functions in terms of power sums, we can easily write the k-statistic in terms of sample moments about the mean.

Because the expressions for k-statistics in terms of augmented symmetric functions and augmented symmetric functions in terms of power sums are often long and complex, these quantities are best expressed in terms of one another via tables such as Tables B2 through B5. For the reader's convenience, we have collected and reproduced many of the relevant tables from the literature in this appendix. These tables are reproduced from four sources. Table E1 is taken from Kendall and Stuart [14], Table E2 is from David and Kendall [13], Table E3 is from Wishart [11], and Table E4 is from Abdel Aty [12].

TABLE E1

Augmented symmetric functions in terms of power sums

Weights 1-6

weight 1 $(1) = [1]$

weight 2

	$[2]$	$[1^2]$
(2)	1	-1
$(1)^2$	1	1

weight 3

	$[3]$	$[21]$	$[1^3]$
(3)	1	-1	2
$(2)(1)$	1	1	-3
$(1)^3$	1	3	1

weight 4

	$[4]$	$[31]$	$[2^2]$	$[21^2]$	$[1^4]$
(4)	1	-1	-1	2	-6
$(3)(1)$	1	1	·	-2	8
$(2)^2$	1	·	1	-1	3
$(2)(1)^2$	1	2	1	1	-6
$(1)^4$	1	4	3	6	1

weight 5

	$[5]$	$[41]$	$[32]$	$[31^2]$	$[2^21]$	$[21^3]$	$[1^5]$
(5)	1	-1	-1	2	2	-6	24
$(4)(1)$	1	1	·	-2	-1	6	-30
$(3)(2)$	1	·	1	-1	-2	5	-20
$(3)(1)^2$	1	2	1	1	·	-3	20
$(2)^2(1)$	1	1	2	·	1	-3	15
$(2)(1)^3$	1	3	4	3	3	1	-10
$(1)^5$	1	5	10	10	15	10	1

weight 6

	$[6]$	$[51]$	$[42]$	$[41^2]$	$[3^2]$	$[321]$	$[31^3]$	$[2^3]$	$[2^21^2]$	$[21^4]$	$[1^6]$
(6)	1	-1	-1	2	-1	2	-6	2	-6	24	-120
$(5)(1)$	1	1	·	-2	·	-1	6	·	4	-24	144
$(4)(2)$	1	·	1	-1	·	-1	3	-3	5	-18	90
$(4)(1)^2$	1	2	1	1	·	·	-3	·	-1	12	-90
$(3)^2$	1	·	·	·	1	-1	2	·	2	-8	40
$(3)(2)(1)$	1	1	1	·	1	1	-3	·	-4	20	-120
$(3)(1)^3$	1	3	3	3	1	3	1	·	·	-4	40
$(2)^3$	1	·	3	·	·	·	·	1	-1	3	-15
$(2)^2(1)^2$	1	2	3	1	2	4	·	1	1	-6	45
$(2)(1)^4$	1	4	7	6	4	16	4	3	6	1	-15
$(1)^6$	1	6	15	15	10	60	20	15	45	15	1

To express the [ ] functions in terms of ( ), read downwards up to and including the main diagonal, e.g. $[41^2] = 2(6) - 2(5)(1) - (4)(2) + (4)(1)^2$. To express the ( ) functions in terms of [ ], read across up to and including the main diagonal, e.g. $(4)(1)^2 = [6] + 2[51] + [42] + [41^2]$.

TABLE E2

Augmented symmetric functions in terms of power sums.

Weights 7 & 8

$w=7$	$[7]$	$[61]$	$[52]$	$[51^2]$	$[43]$	$[421]$	$[41^3]$	$[3^21]$	$[32^2]$	$[321^2]$	$[31^4]$	$[2^31]$	$[2^21^3]$	$[21^5]$	$[1^7]$
(7)	1	−1	−1	2	−1	2	−6	2	2	−6	24	−6	24	−120	720
$(6)(1)$	1	1	.	−2	.	−1	6	−1	.	4	−24	2	−18	120	−840
$(5)(2)$	1	.	1	−1	.	−1	3	.	−2	3	−12	6	−18	84	−504
$(5)(1)^2$	1	2	1	1	.	.	−3	.	.	−1	12	.	6	−60	504
$(4)(3)$	1	.	.	.	1	−1	2	−2	−1	4	−14	3	−14	70	−420
$(4)(2)(1)$	1	1	1	.	1	1	−3	.	.	−2	12	−3	15	−90	630
$(4)(1)^3$	1	3	3	3	1	3	1	.	.	.	−4	.	−1	20	−210
$(3)^2(1)$	1	1	.	.	2	.	.	1	.	−2	8	.	6	−40	280
$(3)(2)^2$	1	.	2	.	1	.	.	.	1	−1	3	−3	8	−35	210
$(3)(2)(1)^2$	1	2	2	1	3	2	.	2	1	1	−6	.	−6	50	−420
$(3)(1)^4$	1	4	6	6	5	12	4	4	3	6	1	.	.	−5	70
$(2)^3(1)$	1	1	3	.	3	3	.	.	3	.	.	1	−3	15	−105
$(2)^2(1)^3$	1	3	5	3	7	9	1	6	7	6	.	3	1	−10	105
$(2)(1)^5$	1	5	11	10	15	35	10	20	25	40	5	15	10	1	−21
$(1)^7$	1	7	21	21	35	105	35	70	105	210	35	105	105	21	1

$w=8$ (i)	$[8]$	$[71]$	$[62]$	$[61^2]$	$[53]$	$[521]$	$[51^3]$	$[4^2]$	$[431]$	$[42^2]$	$[421^2]$	$[41^4]$
(8)	1	−1	−1	2	−1	2	−6	−1	2	2	−6	24
$(7)(1)$	1	1	.	−2	.	−1	6	.	−1	.	4	−24
$(6)(2)$	1	.	1	−1	.	−1	3	.	.	−2	3	−12
$(6)(1)^2$	1	2	1	1	.	.	−3	.	.	.	−1	12
$(5)(3)$	1	.	.	.	1	−1	2	.	−1	.	2	−8
$(5)(2)(1)$	1	1	1	.	1	1	−3	.	.	.	−2	12
$(5)(1)^3$	1	3	3	3	1	3	1	.	.	.	.	−4
$(4)^2$	1	.	.	.	.	.	.	1	−1	−1	2	−6
$(4)(3)(1)$	1	1	.	.	1	.	.	1	1	.	−2	8
$(4)(2)^2$	1	.	2	.	.	.	.	1	.	1	−1	3
$(4)(2)(1)^2$	1	2	2	1	2	2	.	1	2	1	1	−6
$(4)(1)^4$	1	4	6	6	4	12	4	1	4	3	6	1
$(3)^2(2)$	1	.	1	.	2	.	.	.	.	.	.	.
$(3)^2(1)^2$	1	2	1	1	2	.	.	2	4	.	.	.
$(3)(2)^2(1)$	1	1	2	.	3	2	.	1	1	1	.	.
$(3)(2)(1)^3$	1	3	4	3	5	6	1	3	9	3	3	.
$(3)(1)^5$	1	5	10	10	11	30	10	5	25	15	30	5
$(2)^4$	1	.	4	.	.	.	.	3	.	6	.	.
$(2)^3(1)^2$	1	2	4	1	6	6	.	3	6	6	3	.
$(2)^2(1)^4$	1	4	8	6	12	20	4	7	28	16	18	1
$(2)(1)^6$	1	6	16	15	26	66	20	15	90	60	105	15
$(1)^8$	1	8	28	28	56	168	56	35	280	210	420	70

$w=8$ (ii)	$[3^22]$	$[3^21^2]$	$[32^21]$	$[321^3]$	$[31^5]$	$[2^4]$	$[2^31^2]$	$[2^21^4]$	$[21^6]$	$[1^8]$
(8)	2	−6	−6	24	−120	−6	24	−120	720	−5040
$(7)(1)$	.	4	2	−18	120	.	−12	96	−720	5760
$(6)(2)$	−1	1	4	−12	60	8	−20	84	−480	3360
$(6)(1)^2$	.	−1	.	6	−60	.	2	−36	360	−3360
$(5)(3)$	−2	4	4	−14	64	.	−12	64	−384	2688
$(5)(2)(1)$	.	.	−2	9	−60	.	12	−72	504	−4032
$(5)(1)^3$	.	.	.	−1	20	.	.	8	−120	1344
$(4)^2$	.	2	1	−6	30	3	−6	30	−180	1260
$(4)(3)(1)$	.	−4	−1	12	−70	.	6	−56	420	−3360
$(4)(2)^2$	.	.	−1	3	−15	−6	9	−33	180	−1260
$(4)(2)(1)^2$	.	.	.	−3	30	.	−3	30	−270	2520
$(4)(1)^4$	.	.	.	.	−5	.	.	−1	30	−420
$(3)^2(2)$	1	−1	−2	5	−20	.	6	−28	160	−1120
$(3)^2(1)^2$	1	1	.	−3	20	.	.	12	−120	1120
$(3)(2)^2(1)$	2	.	1	−3	15	.	−6	32	−210	1680
$(3)(2)(1)^3$	4	3	3	1	−10	.	.	−8	100	−1120
$(3)(1)^5$	10	10	15	10	1	.	.	.	−6	112
$(2)^4$	.	.	.	.	.	1	−1	3	−15	105
$(2)^3(1)^2$	6	.	6	.	.	1	1	−6	45	−420
$(2)^2(1)^4$	20	12	28	8	.	3	6	1	−15	210
$(2)(1)^6$	70	60	150	80	6	15	45	15	1	−28
$(1)^8$	280	280	840	560	56	105	420	210	28	1

TABLE E3

k-statistics in terms of augmented symmetric functions.

Orders 1-6

1st order $k_1 = [1]/n$

2nd order

	k_{11}	k_2
$[1^2]/n^{(2)}$	*1*	−1
$[2]/n$	1	*1*

3rd order

	k_{111}	k_{21}	k_3
$[1^3]/n^{(3)}$	*1*	−1	2
$[21]/n^{(2)}$	1	*1*	−3
$[3]/n$	1	3	*1*

4th order

	k_{1111}	k_{211}	k_{22}	k_{31}	k_4
$[1^4]/n^{(4)}$	*1*	−1	1	2	−6
$[21^2]/n^{(3)}$	1	*1*	−2	−3	12
$[2^2]/n^{(2)}$	1	2	*1*	.	−3
$[31]/n^{(2)}$	1	3	.	*1*	−4
$[4]/n$	1	6	3	4	*1*

5th order

	k_{11111}	k_{2111}	k_{221}	k_{311}	k_{32}	k_{41}	k_5
$[1^5]/n^{(5)}$	*1*	−1	1	2	−2	−6	24
$[21^3]/n^{(4)}$	1	*1*	−2	−3	5	12	−60
$[2^21]/n^{(3)}$	1	2	*1*	.	−3	−3	30
$[31^2]/n^{(3)}$	1	3	.	*1*	−1	−4	20
$[32]/n^{(2)}$	1	4	3	1	*1*	.	−10
$[41]/n^{(2)}$	1	6	3	4	.	*1*	−5
$[5]/n$	1	10	15	10	10	5	*1*

6th order

	k_{111111}	k_{21111}	k_{2211}	k_{3111}	k_{222}	k_{321}	k_{411}	k_{33}	k_{42}	k_{51}	k_6
$[1^6]/n^{(6)}$	*1*	−1	1	2	−1	−2	−6	4	6	24	−120
$[21^4]/n^{(5)}$	1	*1*	−2	−3	3	5	12	−12	−18	−60	360
$[2^21^2]/n^{(4)}$	1	2	*1*	.	−3	−3	−3	9	15	30	−270
$[31^3]/n^{(4)}$	1	3	.	*1*	.	−1	−4	4	4	20	−120
$[2^3]/n^{(3)}$	1	3	3	.	*1*	.	.	.	−3	.	30
$[321]/n^{(3)}$	1	4	3	1	.	*1*	.	−6	−4	−10	120
$[41^2]/n^{(3)}$	1	6	3	4	.	.	*1*	.	−1	−5	30
$[3^2]/n^{(2)}$	1	6	9	2	.	6	.	*1*	.	.	−10
$[42]/n^{(2)}$	1	7	9	4	3	4	1	.	*1*	.	−15
$[51]/n^{(2)}$	1	10	15	10	.	10	5	.	.	*1*	−6
$[6]/n$	1	15	45	20	15	60	15	10	15	6	*1*

TABLE E4

k-statistics of order 12 in terms of augmented symmetric functions.

Weight 12 (i)	$k_{1^{12}}$	$k_{21^{10}}$	$k_{2^21^8}$	$k_{2^31^6}$	$k_{2^41^4}$	$k_{2^51^2}$	k_{2^6}	k_{31^9}	k_{321^7}	$k_{32^21^5}$	$k_{32^31^3}$	k_{32^41}	$k_{3^21^6}$	$k_{3^221^4}$	$k_{3^22^21^2}$
$[1^{12}]/n^{(12)}$	1	−1	1	−1	1	−1	1	2	−2	2	−2	2	4	−4	4
$[21^{10}]/n^{(11)}$	1	1	−2	3	−4	5	−6	−3	5	−7	9	−11	−12	16	−20
$[2^21^8]/n^{(10)}$	1	2	1	−3	6	−10	15	.	−3	8	−15	24	9	−21	37
$[2^31^6]/n^{(9)}$	1	3	3	1	−4	10	−20	.	.	−3	11	−26	.	9	−30
$[2^41^4]/n^{(8)}$	1	4	6	4	1	−5	15	.	.	.	−3	14	.	.	9
$[2^51^2]/n^{(7)}$	1	5	10	10	5	1	−6	.	.	.	.	−3	.	.	.
$[2^6]/n^{(6)}$	1	6	15	20	15	6	1	.	.	.	.	.	.	.	.
$[31^9]/n^{(10)}$	1	3	.	.	.	.	.	1	−1	1	−1	1	4	−4	4
$[321^7]/n^{(9)}$	1	4	3	.	.	.	.	1	1	−2	3	−4	−6	10	−14
$[32^21^5]/n^{(8)}$	1	5	7	3	.	.	.	1	2	1	−3	6	.	−6	16
$[32^31^3]/n^{(7)}$	1	6	12	10	3	.	.	1	3	3	1	−4	.	.	−6
$[32^41]/n^{(6)}$	1	7	18	22	13	3	.	1	4	6	4	1	.	.	.
$[3^21^6]/n^{(8)}$	1	6	9	.	.	.	.	2	6	.	.	.	1	−1	1
$[3^221^4]/n^{(7)}$	1	7	15	9	.	.	.	2	8	6	.	.	1	1	−2
$[3^22^21^2]/n^{(6)}$	1	8	22	24	9	.	.	2	10	14	6	.	1	2	1
$[3^22^3]/n^{(5)}$	1	9	30	46	33	9	.	2	12	24	20	6	1	3	3
$[3^31^3]/n^{(6)}$	1	9	27	27	.	.	.	3	18	27	.	.	3	9	.
$[3^321]/n^{(5)}$	1	10	36	54	27	.	.	3	21	45	27	.	3	12	9
$[3^4]/n^{(4)}$	1	12	54	108	81	.	.	4	36	108	108	.	6	36	54
$[41^8]/n^{(9)}$	1	6	3	.	.	.	.	4	.	.	.	.	.	.	.
$[421^6]/n^{(8)}$	1	7	9	3	.	.	.	4	4	.	.	.	.	.	.
$[42^21^4]/n^{(7)}$	1	8	16	12	3	.	.	4	8	4	.	.	.	.	.
$[42^31^2]/n^{(6)}$	1	9	24	28	15	3	.	4	12	12	4	.	.	.	.
$[42^4]/n^{(5)}$	1	10	33	52	43	18	3	4	16	24	16	4	.	.	.
$[431^5]/n^{(7)}$	1	9	21	9	.	.	.	5	18	3	.	.	4	.	.
$[4321^3]/n^{(6)}$	1	10	30	30	9	.	.	5	23	21	3	.	4	4	.
$[432^21]/n^{(5)}$	1	11	40	60	39	9	.	5	28	44	24	3	4	8	4
$[43^21^2]/n^{(5)}$	1	12	48	72	27	.	.	6	42	78	18	.	9	30	3
$[43^22]/n^{(4)}$	1	13	60	120	99	27	.	6	48	120	96	18	9	39	33
$[4^21^4]/n^{(6)}$	1	12	42	36	9	.	.	8	48	24	.	.	16	.	.
$[4^221^2]/n^{(5)}$	1	13	54	78	45	9	.	8	56	72	24	.	16	16	.
$[4^22^2]/n^{(4)}$	1	14	67	132	123	54	9	8	64	128	96	24	16	32	16
$[4^231]/n^{(4)}$	1	15	78	162	117	27	.	9	84	210	108	9	24	96	24
$[4^3]/n^{(3)}$	1	18	117	324	351	162	27	12	144	504	432	108	48	288	144
$[51^7]/n^{(8)}$	1	10	15	.	.	.	.	10	10	.	.	.	.	.	.
$[521^5]/n^{(7)}$	1	11	25	15	.	.	.	10	20	10	.	.	.	.	.
$[52^21^3]/n^{(6)}$	1	12	36	40	15	.	.	10	30	30	10	.	.	.	.
$[52^31]/n^{(5)}$	1	13	48	76	55	15	.	10	40	60	40	10	.	.	.
$[531^4]/n^{(6)}$	1	13	45	45	.	.	.	11	50	45	.	.	10	10	.
$[5321^2]/n^{(5)}$	1	14	58	90	45	.	.	11	61	95	45	.	10	20	10
$[532^2]/n^{(4)}$	1	15	72	148	135	45	.	11	72	156	140	45	10	30	30
$[53^21]/n^{(4)}$	1	16	84	180	135	.	.	12	96	240	180	.	21	90	75
$[541^3]/n^{(5)}$	1	16	78	120	45	.	.	14	110	150	30	.	40	40	.
$[5421]/n^{(4)}$	1	17	94	198	165	45	.	14	124	260	180	30	40	80	40
$[543]/n^{(3)}$	1	19	126	354	405	135	.	15	168	558	600	135	54	270	270
$[5^21^2]/n^{(4)}$	1	20	130	300	225	.	.	20	220	500	300	.	100	200	100
$[5^22]/n^{(3)}$	1	21	150	430	525	225	.	20	240	720	800	300	100	300	300
$[61^6]/n^{(7)}$	1	15	45	15	.	.	.	20	60	.	.	.	10	.	.
$[621^4]/n^{(6)}$	1	16	60	60	15	.	.	20	80	60	.	.	10	10	.
$[62^21^2]/n^{(5)}$	1	17	76	120	75	15	.	20	100	140	60	.	10	20	10
$[62^3]/n^{(4)}$	1	18	93	196	195	90	15	20	120	240	200	60	10	30	30
$[631^3]/n^{(5)}$	1	18	90	150	45	.	.	21	135	225	15	.	30	90	.
$[6321]/n^{(4)}$	1	19	108	240	195	45	.	21	156	360	240	15	30	120	90
$[63^2]/n^{(3)}$	1	21	144	420	495	135	.	22	216	720	840	90	51	315	495
$[641^2]/n^{(4)}$	1	21	138	330	225	45	.	24	240	600	240	.	90	300	30
$[642]/n^{(3)}$	1	22	159	468	555	270	45	24	264	840	840	240	90	390	330
$[651]/n^{(3)}$	1	25	210	690	825	225	.	30	420	1500	1500	150	210	900	750
$[6^2]/n^{(2)}$	1	30	315	1380	2475	1350	225	40	720	3600	6000	1800	420	2700	4500
$[71^5]/n^{(6)}$	1	21	105	105	.	.	.	35	210	105	.	.	70	.	.
$[721^3]/n^{(5)}$	1	22	126	210	105	.	.	35	245	315	105	.	70	70	.
$[72^21]/n^{(4)}$	1	23	148	336	315	105	.	35	280	560	420	105	70	140	70
$[731^2]/n^{(4)}$	1	24	168	420	315	.	.	36	336	840	420	.	105	420	105
$[732]/n^{(3)}$	1	25	192	588	735	315	.	36	372	1176	1260	420	105	525	525
$[741]/n^{(3)}$	1	27	234	798	945	315	.	39	504	1890	1680	315	210	1260	630
$[75]/n^{(2)}$	1	31	330	1470	2625	1575	.	45	780	3990	6300	2625	420	3150	4200
$[81^4]/n^{(5)}$	1	28	210	420	105	.	.	56	560	840	.	.	280	280	.
$[821^2]/n^{(4)}$	1	29	238	630	525	105	.	56	616	1400	840	.	280	560	280
$[82^2]/n^{(3)}$	1	30	267	868	1155	630	105	56	672	2016	2240	840	280	840	840
$[831]/n^{(3)}$	1	31	294	1050	1365	315	.	57	756	2730	2940	105	336	1680	1680
$[84]/n^{(2)}$	1	34	381	1764	3255	1890	315	60	1008	5208	8400	2940	504	4200	5880
$[91^3]/n^{(4)}$	1	36	378	1260	945	.	.	84	1260	3780	1260	.	840	2520	.
$[921]/n^{(3)}$	1	37	414	1638	2205	945	.	84	1344	5040	5040	1260	840	3360	2520
$[93]/n^{(2)}$	1	39	486	2394	4725	2835	.	85	1548	7938	13860	4725	924	6300	11340
$[10, 1^2]/n^{(3)}$	1	45	630	3150	4725	945	.	120	2520	12600	12600	.	2100	12600	6300
$[10, 2]/n^{(2)}$	1	46	675	3780	7875	5670	945	120	2640	15120	25200	12600	2100	14700	18900
$[11, 1]/n^{(2)}$	1	55	990	6930	17325	10395	.	165	4620	34650	69300	17325	4620	46200	69300
$[12]/n$	1	66	1485	13860	51975	62370	10395	220	7920	83160	277200	207900	9240	138600	415800

TABLE E4 (continued)

Weight 12 (ii)	$k_{3^2 2^3}$	$k_{3^3 1^3}$	$k_{3^3 21}$	k_{3^4}	k_{41^8}	k_{421^6}	$k_{42^2 1^4}$	$k_{42^3 1^2}$	k_{42^4}	k_{431^5}	k_{4321^3}	$k_{432^2 1}$	$k_{43^2 1^2}$
$[1^{12}]/n^{(12)}$	−4	8	−8	16	−6	6	−6	6	−6	−12	12	−12	−24
$[21^{10}]/n^{(11)}$	24	−36	44	−96	12	−18	24	−30	36	42	−54	66	120
$[2^2 1^8]/n^{(10)}$	−57	54	−90	216	−3	15	−33	57	−87	−42	84	−138	−210
$[2^3 1^6]/n^{(9)}$	67	−27	81	−216	.	−3	18	−51	108	9	−51	135	144
$[2^4 1^4]/n^{(8)}$	−39	.	−27	81	.	.	−3	21	−72	.	9	−60	−27
$[2^5 1^2]/n^{(7)}$	9	.	.	.	.	.	.	−3	24	.	.	9	.
$[2^6]/n^{(6)}$	.	.	.	.	.	.	.	.	−3	.	.	.	.
$[31^9]/n^{(10)}$	−4	12	−12	32	−4	4	−4	4	−4	−14	14	−14	−40
$[321^7]/n^{(9)}$	18	−36	48	−144	.	−4	8	−12	16	24	−38	52	132
$[32^2 1^5]/n^{(8)}$	−30	27	−63	216	.	.	−4	12	−24	−3	27	−65	−120
$[32^3 1^3]/n^{(7)}$	22	.	27	−108	.	.	.	−4	16	.	−3	30	18
$[32^4 1]/n^{(6)}$	−6	.	.	.	.	.	.	.	−4	.	.	−3	.
$[3^2 1^6]/n^{(8)}$	−1	6	−6	24	.	.	.	.	.	−4	4	−4	−22
$[3^2 21^4]/n^{(7)}$	3	−9	15	−72	.	.	.	.	.	.	−4	8	36
$[3^2 2^2 1^2]/n^{(6)}$	−3	.	−9	54	.	.	.	.	.	.	.	−4	−3
$[3^2 2^3]/n^{(5)}$	1	.	.	.	.	.	.	.	.	.	.	.	.
$[3^3 1^3]/n^{(6)}$	.	1	−1	8	.	.	.	.	.	.	.	.	−4
$[3^3 21]/n^{(5)}$	.	1	1	−12	.	.	.	.	.	.	.	.	.
$[3^4]/n^{(4)}$	.	4	12	1	.	.	.	.	.	.	.	.	.
$[41^8]/n^{(9)}$	.	.	.	.	1	−1	1	−1	1	2	−2	2	4
$[421^6]/n^{(8)}$	.	.	.	.	1	1	−2	3	−4	−3	5	−7	−12
$[42^2 1^4]/n^{(7)}$	.	.	.	.	1	2	1	−3	6	.	−3	8	9
$[42^3 1^2]/n^{(6)}$	.	.	.	.	1	3	3	1	−4	.	.	−3	.
$[42^4]/n^{(5)}$	.	.	.	.	1	4	6	4	1	.	.	.	.
$[431^5]/n^{(7)}$	.	.	.	.	1	3	.	.	.	1	−1	−1	4
$[4321^3]/n^{(6)}$	.	.	.	.	1	4	3	.	.	1	1	−2	−6
$[432^2 1]/n^{(5)}$	.	.	.	.	1	5	7	3	.	1	2	1	.
$[43^2 1^2]/n^{(5)}$	.	4	.	.	1	6	9	.	.	2	6	.	1
$[43^2 2]/n^{(4)}$	3	4	4	.	1	7	15	9	.	2	8	6	1
$[4^2 1^4]/n^{(6)}$	.	.	.	.	2	12	6	.	.	8	.	.	.
$[4^2 21^2]/n^{(5)}$	.	.	.	.	2	14	18	6	.	8	8	.	.
$[4^2 2^2]/n^{(4)}$	.	.	.	.	2	16	32	24	6	8	16	8	.
$[4^2 31]/n^{(4)}$	.	16	.	.	2	18	42	18	.	10	36	6	8
$[4^3]/n^{(3)}$	.	64	.	.	3	36	126	108	27	24	144	72	48
$[51^7]/n^{(8)}$	.	.	.	.	5	.	.	.	.	.	.	.	.
$[521^5]/n^{(7)}$	.	.	.	.	5	5	.	.	.	.	.	.	.
$[52^2 1^3]/n^{(6)}$	.	.	.	.	5	10	5	.	.	.	.	.	.
$[52^3 1]/n^{(5)}$	.	.	.	.	5	15	15	5	.	.	.	.	.
$[531^4]/n^{(6)}$	.	.	.	.	5	15	.	.	.	5	.	.	.
$[5321^2]/n^{(5)}$	.	.	.	.	5	20	15	.	.	5	5	.	.
$[532^2]/n^{(4)}$	10	.	.	.	5	25	35	15	.	5	10	5	.
$[53^2 1]/n^{(4)}$	.	10	10	.	5	30	45	.	.	10	30	.	5
$[541^3]/n^{(5)}$	.	.	.	.	6	40	30	.	.	30	10	.	.
$[5421]/n^{(4)}$	.	.	.	.	6	46	70	30	.	30	40	10	.
$[543]/n^{(3)}$	30	40	40	.	6	58	150	90	.	36	140	60	30
$[5^2 1^2]/n^{(4)}$	.	.	.	.	10	100	150	.	.	100	100	.	.
$[5^2 2]/n^{(3)}$	100	.	.	.	10	110	250	150	.	100	200	100	.
$[61^6]/n^{(7)}$	.	.	.	.	15	15	.	.	.	.	.	.	.
$[621^4]/n^{(6)}$	.	.	.	.	15	30	15	.	.	.	.	.	.
$[62^2 1^2]/n^{(5)}$	.	.	.	.	15	45	45	15	.	.	.	.	.
$[62^3]/n^{(4)}$	10	.	.	.	15	60	90	60	15	.	.	.	.
$[631^3]/n^{(5)}$	.	10	.	.	15	60	45	.	.	15	15	.	.
$[6321]/n^{(4)}$	.	10	10	.	15	75	105	45	.	15	30	15	.
$[63^2]/n^{(3)}$	15	40	120	10	15	105	225	135	.	30	120	90	15
$[641^2]/n^{(4)}$	.	40	.	.	16	120	180	60	.	80	120	.	10
$[642]/n^{(3)}$	30	40	40	.	16	136	300	240	60	80	200	120	10
$[651]/n^{(3)}$	.	100	100	.	20	240	600	300	.	250	600	150	50
$[6^2]/n^{(2)}$	300	400	1200	100	30	480	1800	1800	450	600	2400	1800	300
$[71^5]/n^{(6)}$	.	.	.	.	35	105	.	.	.	35	.	.	.
$[721^3]/n^{(5)}$	.	.	.	.	35	140	105	.	.	35	35	.	.
$[72^2 1]/n^{(4)}$	.	.	.	.	35	175	245	105	.	35	70	35	.
$[731^2]/n^{(4)}$	.	70	.	.	35	210	315	.	.	70	210	.	35
$[732]/n^{(3)}$	105	70	70	.	35	245	525	315	.	70	280	210	35
$[741]/n^{(3)}$	.	280	.	.	36	336	840	420	.	210	840	210	210
$[75]/n^{(2)}$	1050	700	700	.	40	560	2100	2100	.	560	2800	2100	700
$[81^4]/n^{(5)}$	.	.	.	.	70	420	210	.	.	280	.	.	.
$[821^2]/n^{(4)}$	.	.	.	.	70	490	630	210	.	280	280	.	.
$[82^2]/n^{(3)}$	280	.	.	.	70	560	1120	840	210	280	560	280	.
$[831]/n^{(3)}$	.	280	280	.	70	630	1470	630	.	350	1260	210	280
$[84]/n^{(2)}$	840	1120	1120	.	71	868	3150	2940	735	616	3920	2520	1400
$[91^3]/n^{(4)}$	.	280	.	.	126	1260	1890	.	.	1260	1260	.	.
$[921]/n^{(3)}$	.	280	280	.	126	1386	3150	1890	.	1260	2520	1260	.
$[93]/n^{(2)}$	1260	1120	3360	280	126	1638	5670	5670	.	1386	6300	5670	1260
$[10, 1^2]/n^{(3)}$	.	2800	.	.	210	3150	9450	3150	.	4200	12600	.	2100
$[10, 2]/n^{(2)}$	6300	2800	2800	.	210	3360	12600	12600	3150	4200	16800	12600	2100
$[11, 1]/n^{(2)}$	.	15400	15400	.	330	6930	34650	34650	.	11550	69300	34650	23100
$[12]/n$	138600	61600	184800	15400	495	13860	103950	207900	51975	27720	277200	415800	138600

TABLE E4 (continued)

Weight 12 (iii)	k_{43^22}	$k_{4^21^4}$	$k_{4^221^2}$	$k_{4^22^2}$	k_{4^231}	k_{4^3}	k_{51^7}	k_{521^5}	$k_{52^21^3}$	k_{52^31}	k_{531^4}	k_{5321^2}	k_{532^2}
$[1^{12}]/n^{(12)}$	24	36	−36	36	72	−216	24	−24	24	−24	48	−48	48
$[21^{10}]/n^{(11)}$	−144	−144	180	−216	−396	1296	−60	84	−108	132	−192	240	−288
$[2^21^8]/n^{(10)}$	330	180	−324	504	792	−2916	30	−90	174	−282	240	−432	672
$[2^31^6]/n^{(9)}$	−354	−72	252	−576	−684	3024	.	30	−120	294	−90	330	−762
$[2^41^4]/n^{(8)}$	171	9	−81	333	234	−1458	.	.	30	−150	.	−90	420
$[2^51^2]/n^{(7)}$	−27	.	9	−90	−27	324	.	.	.	30	.	.	−90
$[2^6]/n^{(6)}$	.	.	.	9	.	−27	.	.	.	.	.	.	.
$[31^9]/n^{(10)}$	40	48	−48	48	132	−432	20	−20	20	−20	64	−64	64
$[321^7]/n^{(9)}$	−172	−96	144	−192	−480	1728	−10	30	−50	70	−140	204	−268
$[32^21^5]/n^{(8)}$	252	24	−120	264	516	−2160	.	−10	40	−90	60	−200	404
$[32^31^3]/n^{(7)}$	−138	.	24	−144	−144	864	.	.	−10	50	.	60	−260
$[32^41]/n^{(6)}$	18	.	.	24	9	−108	.	.	.	−10	.	.	60
$[3^21^6]/n^{(8)}$	22	16	−16	16	80	−288	.	.	.	.	20	−20	20
$[3^221^4]/n^{(7)}$	−58	.	16	−32	−144	576	.	.	.	.	−10	30	−50
$[3^22^21^2]/n^{(6)}$	39	.	.	16	24	−144	.	.	.	.	.	−10	40
$[3^22^3]/n^{(5)}$	−3	.	.	.	.	.	.	.	.	.	.	.	−10
$[3^31^3]/n^{(6)}$	4	.	.	.	16	−64	.	.	.	.	.	.	.
$[3^321]/n^{(5)}$	−4	.	.	.	.	.	.	.	.	.	.	.	.
$[3^4]/n^{(4)}$	.	.	.	.	.	.	.	.	.	.	.	.	.
$[41^8]/n^{(9)}$	−4	−12	12	−12	−24	108	−5	5	−5	5	−10	10	−10
$[421^6]/n^{(8)}$	16	24	−36	48	84	−432	.	−5	10	−15	15	−25	35
$[42^21^4]/n^{(7)}$	−21	−6	30	−66	−84	540	.	.	−5	15	.	15	−40
$[42^31^2]/n^{(6)}$	9	.	−6	36	18	−216	.	.	.	−5	.	.	15
$[42^4]/n^{(5)}$	.	.	.	−6	.	27	.	.	.	.	.	.	.
$[431^5]/n^{(7)}$	−4	−8	8	−8	−28	144	.	.	.	.	−5	5	−5
$[4321^3]/n^{(6)}$	10	.	−8	16	48	−288	.	.	.	.	.	−5	10
$[432^21]/n^{(5)}$	−6	.	.	−8	−6	72	.	.	.	.	.	.	−5
$[43^21^2]/n^{(5)}$	−1	.	.	.	−8	48	.	.	.	.	.	.	.
$[43^22]/n^{(4)}$	*1*	.	.	.	.	.	.	.	.	.	.	.	.
$[4^21^4]/n^{(6)}$	.	*1*	−1	1	2	−18	.	.	.	.	.	.	.
$[4^221^2]/n^{(5)}$	.	1	*1*	−2	−3	36	.	.	.	.	.	.	.
$[4^22^2]/n^{(4)}$	.	1	2	*1*	.	−9	.	.	.	.	.	.	.
$[4^231]/n^{(4)}$	.	1	3	.	*1*	−12	.	.	.	.	.	.	.
$[4^3]/n^{(3)}$	.	3	18	9	12	*1*	.	.	.	.	.	.	.
$[51^7]/n^{(8)}$	.	.	.	.	.	.	*1*	−1	1	−1	2	−2	2
$[521^5]/n^{(7)}$	.	.	.	.	.	.	1	*1*	−2	3	−3	5	−7
$[52^21^3]/n^{(6)}$	.	.	.	.	.	.	1	2	*1*	−3	.	−3	8
$[52^31]/n^{(5)}$	.	.	.	.	.	.	1	3	3	*1*	.	.	−3
$[531^4]/n^{(6)}$	.	.	.	.	.	.	1	3	.	.	*1*	−1	1
$[5321^2]/n^{(5)}$	.	.	.	.	.	.	1	4	3	.	1	*1*	−2
$[532^2]/n^{(4)}$	.	.	.	.	.	.	1	5	7	3	1	2	*1*
$[53^21]/n^{(4)}$	.	.	.	.	.	.	1	6	9	.	2	6	.
$[541^3]/n^{(5)}$	.	5	.	.	.	.	1	6	3	.	4	.	.
$[5421]/n^{(4)}$	.	5	5	.	.	.	1	7	9	3	4	4	.
$[543]/n^{(3)}$	10	5	15	.	5	.	1	9	21	9	5	18	3
$[5^21^2]/n^{(4)}$	.	25	.	.	.	.	2	20	30	.	20	20	.
$[5^22]/n^{(3)}$	.	25	25	.	.	.	2	22	50	30	20	40	20
$[61^6]/n^{(7)}$	.	.	.	.	.	.	6	.	.	.	.	.	.
$[621^4]/n^{(6)}$	.	.	.	.	.	.	6	6	.	.	.	.	.
$[62^21^2]/n^{(5)}$	.	.	.	.	.	.	6	12	6	.	.	.	.
$[62^3]/n^{(4)}$	.	.	.	.	.	.	6	18	18	6	.	.	.
$[631^3]/n^{(5)}$	.	.	.	.	.	.	6	18	.	.	6	.	.
$[6321]/n^{(4)}$	.	.	.	.	.	.	6	24	18	.	6	6	.
$[63^2]/n^{(3)}$	15	.	.	.	.	.	6	36	54	.	12	36	.
$[641^2]/n^{(4)}$	.	15	15	.	.	.	6	36	18	.	24	.	.
$[642]/n^{(3)}$	10	15	30	15	.	.	6	42	54	18	24	24	.
$[651]/n^{(3)}$	.	75	75	.	.	.	7	75	135	15	80	120	.
$[6^2]/n^{(2)}$	300	225	450	225	.	.	12	180	540	180	240	720	.
$[71^5]/n^{(6)}$	.	.	.	.	.	.	21	21	.	.	.	.	.
$[721^3]/n^{(5)}$	.	.	.	.	.	.	21	42	21	.	.	.	.
$[72^21]/n^{(4)}$	.	.	.	.	.	.	21	63	63	21	.	.	.
$[731^2]/n^{(4)}$	.	.	.	.	.	.	21	84	63	.	21	21	.
$[732]/n^{(3)}$	35	.	.	.	.	.	21	105	147	63	21	42	21
$[741]/n^{(3)}$	.	35	105	.	35	.	21	147	189	63	84	84	.
$[75]/n^{(2)}$	350	175	525	.	175	.	22	252	630	420	245	630	315
$[81^4]/n^{(5)}$	.	35	.	.	.	.	56	168	.	.	56	.	.
$[821^2]/n^{(4)}$	.	35	35	.	.	.	56	224	168	.	56	56	.
$[82^2]/n^{(3)}$	.	35	70	35	.	.	56	280	392	168	56	112	56
$[831]/n^{(3)}$	.	35	105	.	35	.	56	336	504	.	112	336	.
$[84]/n^{(2)}$	280	105	630	315	420	35	56	504	1176	504	280	1008	168
$[91^3]/n^{(4)}$	.	315	.	.	.	.	126	756	378	.	504	.	.
$[921]/n^{(3)}$	.	315	315	.	.	.	126	882	1134	378	504	504	.
$[93]/n^{(2)}$	1260	315	945	.	315	.	126	1134	2646	1134	630	2268	378
$[10, 1^2]/n^{(3)}$	.	1575	1575	.	.	.	252	2520	3780	.	2520	2520	.
$[10, 2]/n^{(2)}$	2100	1575	3150	1575	.	.	252	2772	6300	3780	2520	5040	2520
$[11, 1]/n^{(2)}$	.	5775	17325	.	5775	.	462	6930	20790	6930	9240	27720	.
$[12]/n$	138600	17325	103950	51975	69300	5775	792	16632	83160	83160	27720	166320	83160

TABLE E4 (continued)

Weight 12 (iv)	k_{60^21}	k_{641^2}	k_{6421}	k_{642}	$k_{6^21^2}$	k_{6^22}	k_{61^6}	k_{621^4}	$k_{62^21^2}$	k_{62^3}	k_{631^3}	k_{6321}	k_{63^2}
$[1^{12}]/n^{(12)}$	96	−144	144	−288	576	−576	−120	120	−120	120	−240	240	−480
$[21^{10}]/n^{(11)}$	−528	648	−792	1728	−2880	3456	360	−480	600	−720	1080	−1320	2880
$[2^21^8]/n^{(10)}$	1056	−972	1620	−3888	5040	−7920	−270	630	−1110	1710	−1620	2700	−6480
$[2^31^6]/n^{(9)}$	−900	540	−1512	3996	−3600	8640	30	−300	930	−2040	870	−2490	6600
$[2^41^4]/n^{(8)}$	270	−90	630	−1800	900	−4500	.	30	−330	1260	−90	960	−2790
$[2^51^2]/n^{(7)}$	.	.	−90	270	.	900	.	.	30	−360	.	−90	270
$[2^6]/n^{(6)}$	.	.	.	.	.	.	.	.	.	30	.	.	.
$[31^9]/n^{(10)}$	176	−216	216	−576	960	−960	−120	120	−120	120	−360	360	−960
$[321^7]/n^{(9)}$	−664	540	−756	2376	−2880	3840	120	−240	360	−480	960	−1320	4080
$[32^21^5]/n^{(8)}$	780	−300	840	−3192	2400	−5280	.	120	−360	720	−630	1590	−5760
$[32^31^3]/n^{(7)}$	−270	30	−330	1500	−600	3000	.	.	120	−480	30	−660	2820
$[32^41]/n^{(6)}$	.	.	30	−180	.	−600	.	.	.	120	.	30	−180
$[3^21^6]/n^{(8)}$	104	−80	80	−376	400	−400	−10	10	−10	10	−140	140	−640
$[3^221^4]/n^{(7)}$	−220	40	−120	860	−400	800	.	−10	20	−30	150	−290	1680
$[3^22^21^2]/n^{(6)}$	90	.	40	−420	100	−500	.	.	−10	30	.	150	−1080
$[3^22^3]/n^{(5)}$	.	.	.	30	.	100	.	.	.	−10	.	.	30
$[3^31^3]/n^{(6)}$	20	.	.	−80	.	.	.	.	.	.	−10	10	−160
$[3^321]/n^{(5)}$	−10	.	.	40	.	.	.	.	.	.	.	−10	180
$[3^4]/n^{(4)}$	.	.	.	.	.	.	.	.	.	.	.	.	−10
$[41^8]/n^{(9)}$	−20	54	−54	108	−240	240	30	−30	30	−30	60	−60	120
$[421^6]/n^{(8)}$	60	−120	174	−402	600	−840	−15	45	−75	105	−120	180	−420
$[42^21^4]/n^{(7)}$	−45	45	−165	450	−300	900	.	−15	60	−135	45	−165	450
$[42^31^2]/n^{(6)}$	.	.	45	−135	.	−300	.	.	−15	75	.	45	−135
$[42^4]/n^{(5)}$	.	.	.	.	.	.	.	.	.	−15	.	.	.
$[431^5]/n^{(7)}$	−20	40	−40	134	−200	200	.	.	.	.	30	−30	120
$[4321^3]/n^{(6)}$	30	−10	50	−260	100	−300	.	.	.	.	−15	45	−240
$[432^21]/n^{(5)}$	.	.	−10	75	.	100	.	.	.	.	.	−15	90
$[43^21^2]/n^{(5)}$	−5	.	.	40	.	.	.	.	.	.	.	.	30
$[43^22]/n^{(4)}$	.	.	.	−10	.	.	.	.	.	.	.	.	−15
$[4^21^4]/n^{(6)}$	.	−5	5	−10	25	−25	.	.	.	.	.	.	.
$[4^221^2]/n^{(5)}$	.	.	−5	15	.	25	.	.	.	.	.	.	.
$[4^22^2]/n^{(4)}$	.	.	.	.	.	.	.	.	.	.	.	.	.
$[4^231]/n^{(4)}$	.	.	.	−5	.	.	.	.	.	.	.	.	.
$[4^3]/n^{(3)}$	.	.	.	.	.	.	.	.	.	.	.	.	.
$[51^7]/n^{(8)}$	4	−6	6	−12	48	−48	−6	6	−6	6	−12	12	−24
$[521^5]/n^{(7)}$	−12	12	−18	42	−120	168	.	−6	12	−18	18	−30	72
$[52^21^3]/n^{(6)}$	9	−3	15	−42	60	−180	.	.	−6	18	.	18	−54
$[52^31]/n^{(5)}$	.	.	−3	9	.	60	.	.	.	−6	.	.	.
$[531^4]/n^{(6)}$	4	−4	4	−14	40	−40	.	.	.	.	−6	6	−24
$[5321^2]/n^{(5)}$	−6	.	−4	24	−20	60	.	.	.	.	.	−6	36
$[532^2]/n^{(4)}$	.	.	.	−3	.	−20	.	.	.	.	.	.	.
$[53^21]/n^{(4)}$	1	.	.	−4	.	.	.	.	.	.	.	.	−6
$[541^3]/n^{(5)}$	.	1	−1	2	−10	10	.	.	.	.	.	.	.
$[5421]/n^{(4)}$	.	1	1	−3	.	−10	.	.	.	.	.	.	.
$[543]/n^{(3)}$	4	1	3	1	.	.	.	.	.	.	.	.	.
$[5^21^2]/n^{(4)}$	.	10	.	.	1	−1	.	.	.	.	.	.	.
$[5^22]/n^{(3)}$	.	10	10	.	1	1	.	.	.	.	.	.	.
$[61^6]/n^{(7)}$	.	.	.	.	.	.	1	−1	1	−1	2	−2	4
$[621^4]/n^{(6)}$	.	.	.	.	.	.	1	1	−2	3	−3	5	−12
$[62^21^2]/n^{(5)}$	.	.	.	.	.	.	1	2	1	−3	.	−3	9
$[62^3]/n^{(4)}$	.	.	.	.	.	.	1	3	3	1	.	.	.
$[631^3]/n^{(5)}$	.	.	.	.	.	.	1	3	.	.	1	−1	4
$[6321]/n^{(4)}$	.	.	.	.	.	.	1	4	3	.	1	1	−6
$[63^2]/n^{(3)}$	6	.	.	.	.	.	1	6	9	.	2	6	1
$[641^2]/n^{(4)}$	.	6	.	.	.	.	1	6	3	.	4	.	.
$[642]/n^{(3)}$	.	6	6	.	.	.	1	7	9	3	4	4	.
$[651]/n^{(3)}$	10	45	15	.	6	.	1	10	15	.	10	10	.
$[6^2]/n^{(2)}$	120	180	180	.	36	.	2	30	90	30	40	120	20
$[71^5]/n^{(6)}$	.	.	.	.	.	.	7	.	.	.	.	.	.
$[721^3]/n^{(5)}$	.	.	.	.	.	.	7	7	.	.	.	.	.
$[72^21]/n^{(4)}$	.	.	.	.	.	.	7	14	7	.	.	.	.
$[731^2]/n^{(4)}$	.	.	.	.	.	.	7	21	.	.	7	.	.
$[732]/n^{(3)}$	.	.	.	.	.	.	7	28	21	.	7	7	.
$[741]/n^{(3)}$	.	21	21	.	.	.	7	42	21	.	28	.	.
$[75]/n^{(2)}$	70	140	210	35	21	21	7	70	105	.	70	70	.
$[81^4]/n^{(5)}$	.	.	.	.	.	.	28	28	.	.	.	.	.
$[821^2]/n^{(4)}$	.	.	.	.	.	.	28	56	28	.	.	.	.
$[82^2]/n^{(3)}$	.	.	.	.	.	.	28	84	84	28	.	.	.
$[831]/n^{(3)}$	56	.	.	.	.	.	28	112	84	.	28	28	.
$[84]/n^{(2)}$	224	56	168	56	.	.	28	196	252	84	112	112	.
$[91^3]/n^{(4)}$	.	126	.	.	.	.	84	252	.	.	84	.	.
$[921]/n^{(3)}$	.	126	126	.	.	.	84	336	252	.	84	84	.
$[93]/n^{(2)}$	504	126	378	126	.	.	84	504	756	.	168	504	84
$[10, 1^2]/n^{(3)}$	.	1260	.	.	126	.	210	1260	630	.	840	.	.
$[10, 2]/n^{(2)}$	.	1260	1260	.	126	126	210	1470	1890	630	840	840	.
$[11, 1]/n^{(2)}$	4620	6930	6930	.	1386	.	462	4620	6930	.	4620	4620	.
$[12]/n$	55440	27720	83160	27720	8316	8316	924	13860	41580	13860	18480	55440	9240

TABLE E4 (continued)

Weight 12 (v)	k_{641^2}	k_{642}	k_{651}	k_{6^2}	k_{71^5}	k_{721^3}	k_{72^21}	k_{731^2}	k_{732}	k_{741}	k_{75}	k_{81^4}	k_{821^2}
$[1^{12}]/n^{(12)}$	720	−720	−2880	14400	720	−720	720	1440	−1440	−4320	17280	−5040	5040
$[21^{10}]/n^{(11)}$	−3600	4320	15840	−86400	−2520	3240	−3960	−7200	8640	23760	−103680	20160	−25200
$[2^21^8]/n^{(10)}$	6300	−9900	−31680	194400	2520	−5040	8280	12600	−19800	−47520	233280	−25200	45360
$[2^31^6]/n^{(9)}$	−4500	10800	27720	−201600	−630	3150	−8190	−8820	21420	41580	−241920	10080	−35280
$[2^41^4]/n^{(8)}$	1170	−5670	−9900	94500	.	−630	3780	1890	−10710	−15120	113400	−630	10710
$[2^51^2]/n^{(7)}$	−90	1260	900	−16200	.	.	−630	.	1890	1890	−18900	.	−630
$[2^6]/n^{(6)}$	.	−90	.	900	.	.	.	.	.	.	.	.	.
$[31^9]/n^{(10)}$	1200	−1200	−5280	28800	840	−840	840	2400	−2400	−7920	34560	−6720	6720
$[321^7]/n^{(9)}$	−3600	4800	18480	−115200	−1260	2100	−2940	−7560	9960	27720	−138240	13440	−20160
$[32^21^5]/n^{(8)}$	2880	−6480	−19800	151200	210	−1470	3570	6720	−14280	−28980	181440	−5040	18480
$[32^31^3]/n^{(7)}$	−480	3360	6900	−72000	.	210	−1680	−1260	7980	8820	−88200	.	−5040
$[32^41]/n^{(6)}$	.	−480	−300	7200	.	.	210	.	−1260	−630	12600	.	.
$[3^21^6]/n^{(8)}$	540	−540	−2640	16800	140	−140	140	1120	−1120	−4200	20160	−1680	1680
$[3^221^4]/n^{(7)}$	−600	1140	4200	−36000	.	140	−280	−1680	2800	6720	−42000	560	−2240
$[3^22^21^2]/n^{(6)}$	30	−630	−1500	19800	.	.	140	210	−1890	−1260	21000	.	560
$[3^22^3]/n^{(5)}$	.	30	.	−600	.	.	.	.	210	.	−2100	.	.
$[3^31^3]/n^{(6)}$	40	−40	−200	2400	.	.	.	140	−140	−560	2800	.	.
$[3^321]/n^{(5)}$	.	40	109	−2400	.	.	.	.	140	.	−1400	.	.
$[3^4]/n^{(4)}$	.	.	.	100	.	.	.	.	.	.	.	.	.
$[41^8]/n^{(9)}$	−300	300	1320	−7200	−210	210	−210	−420	420	1980	−8640	1680	−1680
$[421^6]/n^{(8)}$	810	−1110	−3960	25200	210	−420	630	1050	−1470	−6300	30240	−2520	4200
$[42^21^4]/n^{(7)}$	−540	1350	3150	−27000	.	210	−630	−630	1680	5670	−31500	420	−2940
$[42^31^2]/n^{(6)}$	75	−615	−600	9900	.	.	210	.	−630	−1260	9450	.	420
$[42^4]/n^{(5)}$	.	75	.	−900	.	.	.	.	.	.	.	.	.
$[431^5]/n^{(7)}$	−240	240	1200	−7200	−35	35	−35	−280	280	1890	−9240	560	−560
$[4321^3]/n^{(6)}$	180	−420	−1200	10800	.	−35	70	315	−595	−2520	14700	.	560
$[432^21]/n^{(5)}$	.	180	150	−3600	.	.	−35	.	315	315	−4200	.	.
$[43^21^2]/n^{(5)}$	−10	10	50	−600	.	.	.	−35	35	280	−1400	.	.
$[43^22]/n^{(4)}$	.	−10	.	300	.	.	.	.	−35	.	350	.	.
$[4^21^4]/n^{(6)}$	30	−30	−150	900	.	.	.	.	.	−210	1050	−35	35
$[4^221^2]/n^{(5)}$	−15	45	75	−900	.	.	.	.	.	210	−1050	.	−35
$[4^22^2]/n^{(4)}$	.	−15	.	225	.	.	.	.	.	.	.	.	.
$[4^231]/n^{(4)}$	.	.	.	.	.	.	.	.	.	−35	175	.	.
$[4^3]/n^{(3)}$	.	.	.	.	.	.	.	.	.	.	.	.	.
$[51^7]/n^{(8)}$	36	−36	−264	1440	42	−42	42	84	−84	−252	1728	−336	336
$[521^5]/n^{(7)}$	−72	108	720	−4320	−21	63	−105	−168	252	630	−5544	336	−672
$[52^21^3]/n^{(6)}$	18	−90	−450	3240	.	−21	84	63	−231	−378	5040	.	336
$[52^31]/n^{(5)}$	.	18	30	−360	.	.	−21	.	63	63	−1260	.	.
$[531^4]/n^{(6)}$	24	−24	−240	1440	.	.	.	42	−42	−168	1680	−56	56
$[5321^2]/n^{(5)}$	.	24	180	−1440	.	.	.	−21	63	84	−2100	.	−56
$[532^2]/n^{(4)}$	.	.	.	.	.	.	.	.	−21	.	420	.	.
$[53^21]/n^{(4)}$	.	.	−10	120	.	.	.	.	.	.	140	.	.
$[541^3]/n^{(5)}$	−6	6	60	−360	.	.	.	.	.	42	−420	.	.
$[5421]/n^{(4)}$	.	−6	−15	180	.	.	.	.	.	−21	315	.	.
$[543]/n^{(3)}$	.	.	.	.	.	.	.	.	.	.	−35	.	.
$[5^21^2]/n^{(4)}$	.	.	−6	36	.	.	.	.	.	.	42	.	.
$[5^22]/n^{(3)}$	.	.	.	.	.	.	.	.	.	.	−21	.	.
$[61^6]/n^{(7)}$	−6	6	24	−240	−7	7	−7	−14	14	42	−168	56	−56
$[621^4]/n^{(6)}$	12	−18	−60	720	.	−7	14	21	−35	−84	420	−28	84
$[62^21^2]/n^{(5)}$	−3	15	30	−540	.	.	−7	.	21	21	−210	.	−28
$[62^3]/n^{(4)}$	.	−3	.	60	.	.	.	.	.	.	.	.	.
$[631^3]/n^{(5)}$	−4	4	20	−240	.	.	.	−7	7	28	−140	.	.
$[6321]/n^{(4)}$	.	−4	−10	240	.	.	.	.	−7	.	70	.	.
$[63^2]/n^{(3)}$	.	.	.	−20	.	.	.	.	.	.	.	.	.
$[641^2]/n^{(4)}$	1	−1	−5	60	.	.	.	.	.	−7	35	.	.
$[642]/n^{(3)}$	1	1	.	−30	.	.	.	.	.	.	.	.	.
$[651]/n^{(3)}$	5	.	1	−12	.	.	.	.	.	.	−7	.	.
$[6^2]/n^{(2)}$	30	30	12	1	.	.	.	.	.	.	.	.	.
$[71^5]/n^{(6)}$	.	.	.	.	1	−1	1	2	−2	−6	24	−8	8
$[721^3]/n^{(5)}$	.	.	.	.	1	1	−2	−3	5	12	−60	.	−8
$[72^21]/n^{(4)}$	.	.	.	.	1	2	1	.	−3	−3	30	.	.
$[731^2]/n^{(4)}$	.	.	.	.	1	3	.	1	−1	−4	20	.	.
$[732]/n^{(3)}$	.	.	.	.	1	4	3	1	1	.	−10	.	.
$[741]/n^{(3)}$	7	.	.	.	1	6	3	4	.	1	−5	.	.
$[75]/n^{(2)}$	35	.	7	.	1	10	15	10	10	5	1	.	.
$[81^4]/n^{(5)}$	.	.	.	.	8	.	.	.	.	.	.	1	−1
$[821^2]/n^{(4)}$	.	.	.	.	8	8	.	.	.	.	.	1	1
$[82^2]/n^{(3)}$	.	.	.	.	8	16	8	.	.	.	.	1	2
$[831]/n^{(3)}$	.	.	.	.	8	24	.	8	.	.	.	1	3
$[84]/n^{(2)}$	28	28	.	.	8	48	24	32	.	8	.	1	6
$[91^3]/n^{(4)}$	.	.	.	.	36	36	.	.	.	.	.	9	.
$[921]/n^{(3)}$	.	.	.	.	36	72	36	.	.	.	.	9	9
$[93]/n^{(2)}$	.	.	.	.	36	144	108	36	36	.	.	9	27
$[10,1^2]/n^{(3)}$	210	.	.	.	120	360	.	120	.	.	.	45	45
$[10,2]/n^{(2)}$	210	210	.	.	120	480	360	120	120	.	.	45	90
$[11,1]/n^{(2)}$	2310	.	462	.	330	1980	990	1320	.	330	.	165	495
$[12]/n$	13860	13860	5544	462	792	7920	11880	7920	7920	3960	792	495	2970

TABLE E4 (continued)

Weight 12 (vi)	k_{82^2}	k_{831}	k_{84}	k_{91^3}	k_{921}	k_{93}	$k_{10,1^2}$	$k_{10,2}$	$k_{11,1}$	k_{12}
$[1^{12}]/n^{(12)}$	-5040	-10080	30240	40320	-40320	80640	-362880	362880	3628800	-39916800
$[21^{10}]/n^{(11)}$	30240	55440	-181440	-181440	221760	-483840	1814400	-2177280	-19958400	239500800
$[2^21^8]/n^{(10)}$	-70560	-110880	408240	272160	-453600	1088640	-3175200	4989600	39916800	-538876800
$[2^31^6]/n^{(9)}$	80640	95760	-423360	-151200	423360	-1118880	2268000	-5443200	-34927200	558835200
$[2^41^4]/n^{(8)}$	-45990	-31500	200340	22680	-173880	498960	-567000	2835000	12474000	-261954000
$[2^51^2]/n^{(7)}$	11340	1890	-37800	.	22680	-68040	22680	-589680	-1247400	44906400
$[2^6]/n^{(6)}$	-630	.	1890	.	.	.	.	22680	.	-1247400
$[31^9]/n^{(10)}$	-6720	-18480	60480	60480	-60480	161280	-604800	604800	6652800	-79833600
$[321^7]/n^{(9)}$	26880	67200	-241920	-151200	211680	-665280	1814400	-2419200	-23284800	319334400
$[32^21^5]/n^{(8)}$	-38640	-75600	312480	90720	-241920	907200	-1512000	3326400	24948000	-419126400
$[32^31^3]/n^{(7)}$	23520	25200	-141120	-7560	98280	-438480	302400	-1814400	-8316000	199584000
$[32^41]/n^{(6)}$	-5040	-630	17640	.	-7560	45360	.	302400	415800	-24948000
$[3^21^6]/n^{(8)}$	-1680	-10080	36960	20160	-20160	100800	-252000	252000	3326400	-46569600
$[3^221^4]/n^{(7)}$	3920	19600	-77280	-15120	35280	-241920	302400	-554400	-5544000	99792000
$[3^22^21^2]/n^{(6)}$	-2800	-6720	31920	.	-15120	136080	-37800	340200	1663200	-49896000
$[3^22^3]/n^{(5)}$	560	.	-1680	.	.	-7560	.	-37800	.	3326400
$[3^31^3]/n^{(6)}$	.	-1680	6720	560	-560	21280	-16800	16800	369600	-7392000
$[3^321]/n^{(5)}$	.	560	-2240	.	560	-16800	.	-16800	-92400	4435200
$[3^4]/n^{(4)}$	.	.	.	.	.	560	.	.	.	-92400
$[41^8]/n^{(9)}$	1680	3360	15120	-15120	15120	-30240	151200	-151200	-1663200	19958400
$[421^6]/n^{(8)}$	-5880	-10080	55440	30240	-45360	105840	-378000	529200	4989600	-69854400
$[42^21^4]/n^{(7)}$	7140	8400	-63000	-11340	41580	-113400	226800	-604800	-4158000	74844000
$[42^31^2]/n^{(6)}$	-3360	-1260	22680	.	-11340	34020	-18900	245700	831600	-24948000
$[42^4]/n^{(5)}$	420	.	-1890	.	.	.	.	-18900	.	1247400
$[431^5]/n^{(7)}$	560	2800	-16800	-7560	7560	-30240	100800	-100800	-1386000	19958400
$[4321^3]/n^{(6)}$	-1120	-4200	30240	2520	-10080	57960	-75600	176400	1663200	-33264000
$[432^21]/n^{(5)}$	560	420	-8400	.	2520	-18900	.	-75600	-207900	9979200
$[43^21^2]/n^{(5)}$	.	560	-3920	.	.	-7560	4200	-4200	-138600	3326400
$[43^22]/n^{(4)}$	.	.	560	.	.	2520	.	4200	.	-831600
$[4^21^4]/n^{(6)}$	-35	-70	1890	630	-630	1260	-9450	9450	138600	-2079000
$[4^221^2]/n^{(5)}$	70	105	-2940	.	630	-1890	3150	-12600	-103950	2494800
$[4^22^2]/n^{(4)}$	-35	.	525	.	.	.	.	3150	.	-311850
$[4^231]/n^{(4)}$	.	-35	700	.	.	630	.	.	11550	-415800
$[4^3]/n^{(3)}$	.	.	-35	.	.	.	.	.	.	11550
$[51^7]/n^{(8)}$	-336	-672	2016	3024	-3024	6048	-30240	30240	332640	-3991680
$[521^5]/n^{(7)}$	1008	1680	-6048	-4536	7560	-18144	60480	-90720	-831600	11975040
$[52^21^3]/n^{(6)}$	-1008	-1008	5040	756	-5292	15120	-22680	83160	498960	-9979200
$[52^31]/n^{(5)}$	336	.	-1008	.	756	-2268	.	-22680	-41580	1995840
$[531^4]/n^{(6)}$	-56	-448	1680	1008	-1008	5040	-15120	15120	221760	-3326400
$[5321^2]/n^{(5)}$	112	504	-2016	.	1008	-7560	5040	-20160	-166320	3991680
$[532^2]/n^{(4)}$	-56	.	168	.	.	756	.	5040	.	-498960
$[53^21]/n^{(4)}$	.	-56	224	.	.	1008	.	.	9240	-332640
$[541^3]/n^{(5)}$	.	.	-336	-126	126	-252	2520	-2520	-41580	665280
$[5421]/n^{(4)}$	.	.	336	.	-126	378	.	2520	13860	-498960
$[543]/n^{(3)}$	.	.	-56	.	.	-126	.	.	.	55440
$[5^21^2]/n^{(4)}$	.	.	.	.	.	.	-126	126	2772	-49896
$[5^22]/n^{(3)}$	.	.	.	.	.	.	.	-126	.	16632
$[61^6]/n^{(7)}$	56	112	-336	-504	504	-1008	5040	-5040	-55440	665280
$[621^4]/n^{(6)}$	-140	-224	840	504	-1008	2520	-7560	12600	110880	-1663200
$[62^21^2]/n^{(5)}$	112	84	-504	.	504	-1512	1260	-8820	-41580	997920
$[62^3]/n^{(4)}$	-28	.	84	.	.	.	.	1260	.	-83160
$[631^3]/n^{(5)}$	.	56	-224	-84	84	-672	1680	-1680	-27720	443520
$[6321]/n^{(4)}$	.	-28	112	.	-84	756	.	1680	9240	-332640
$[63^2]/n^{(3)}$	.	.	.	.	.	-84	.	.	.	18480
$[641^2]/n^{(4)}$	.	.	56	.	.	.	-210	210	4620	-83160
$[642]/n^{(3)}$	.	.	-28	.	.	.	.	-210	.	27720
$[651]/n^{(3)}$	.	.	.	.	.	.	.	.	-462	11088
$[6^2]/n^{(2)}$	.	.	.	.	.	.	.	.	.	-462
$[71^5]/n^{(6)}$	-8	-16	48	72	-72	144	-720	720	7920	-95040
$[721^3]/n^{(5)}$	16	24	-96	-36	108	-288	720	-1440	-11880	190080
$[72^21]/n^{(4)}$	-8	.	24	.	-36	108	.	720	1980	-71280
$[731^2]/n^{(4)}$	.	-8	32	.	.	72	-120	120	2640	-47520
$[732]/n^{(3)}$	.	.	.	.	.	-36	.	-120	.	15840
$[741]/n^{(3)}$	.	.	-8	.	.	.	.	.	-330	7920
$[75]/n^{(2)}$	.	.	.	.	.	.	.	.	.	-792
$[81^4]/n^{(5)}$	1	2	-6	-9	9	-18	90	-90	-990	11880
$[821^2]/n^{(4)}$	-2	-3	12	.	-9	27	-45	135	990	-17820
$[82^2]/n^{(3)}$	1	.	-3	.	.	.	.	-45	.	2970
$[831]/n^{(3)}$	.	1	-4	.	.	-9	.	.	-165	3960
$[84]/n^{(2)}$	3	4	1	.	.	.	.	.	.	-495
$[91^3]/n^{(4)}$	.	.	.	1	-1	2	-10	10	110	-1320
$[921]/n^{(3)}$	.	.	.	1	1	-3	.	-10	-55	1320
$[93]/n^{(2)}$	.	9	.	1	3	1	.	.	.	-220
$[10,1^2]/n^{(3)}$	.	.	.	10	.	.	1	-1	-11	132
$[10,2]/n^{(2)}$	45	.	.	10	10	.	1	1	.	-66
$[11,1]/n^{(2)}$	.	165	.	55	55	.	11	.	1	-12
$[12]/n$	1485	1980	495	220	660	220	66	66	12	1

APPENDIX F

FORMULAE FOR POWERS AND PRODUCTS OF k-STATISTICS, ORDERS 2-8.[11]

2nd order

$$k_1^2 = k_2/n + k_{11}$$

3rd order

$$k_2 k_1 = k_3/n + k_{21},$$
$$k_1^3 = k_3/n^2 + 3k_{21}/n + k_{111},$$
$$k_{11} k_1 = 2k_{21}/n + k_{111}.$$

4th order

$$k_3 k_1 = k_4/n + k_{31},$$
$$k_2^2 = k_4/n + (n+1)\,k_{22}/(n-1),$$
$$k_2 k_1^2 = k_4/n^2 + 2k_{31}/n + k_{22}/n + k_{211},$$
$$k_1^4 = k_4/n^3 + 4k_{31}/n^2 + 3k_{22}/n^2 + 6k_{211}/n + k_{1111}.$$
$$k_{21} k_1 = k_{31}/n + k_{22}/n + k_{211},$$
$$k_2 k_{11} = 2k_{31}/n - 2k_{22}/n^{(2)} + k_{211},$$
$$k_{11} k_1^2 = 2k_{31}/n^2 + 2k_{22}/n^2 + 5k_{211}/n + k_{1111},$$
$$k_{111} k_1 = 3k_{211}/n + k_{1111},$$
$$k_{11}^2 = 2k_{22}/n^{(2)} + 4k_{211}/n + k_{1111}.$$

5th order

$$k_4 k_1 = k_5/n + k_{41},$$
$$k_3 k_2 = k_5/n + (n+5)\,k_{32}/(n-1),$$
$$k_3 k_1^2 = k_5/n^2 + 2k_{41}/n + k_{32}/n + k_{311},$$
$$k_2^2 k_1 = k_5/n^2 + k_{41}/n + 2(n+1)\,k_{32}/n^{(2)} + (n+1)\,k_{221}/(n-1),$$
$$k_2 k_1^3 = k_5/n^3 + 3k_{41}/n^2 + 4k_{32}/n^2 + 3k_{311}/n + 3k_{221}/n + k_{2111},$$
$$k_1^5 = k_5/n^4 + 5k_{41}/n^3 + 10k_{32}/n^3 + 10k_{311}/n^2 + 15k_{221}/n^2 + 10k_{2111}/n + k_{11111}.$$
$$k_{31} k_1 = k_{41}/n + k_{32}/n + k_{311},$$
$$k_3 k_{11} = 2k_{41}/n - 6k_{32}/n^{(2)} + k_{311},$$
$$k_{22} k_1 = 2k_{32}/n + k_{221},$$
$$k_{21} k_2 = k_{41}/n + (n-3)\,k_{32}/n^{(2)} + (n+1)\,k_{221}/(n-1),$$
$$k_{21} k_1^2 = k_{41}/n^2 + 3k_{32}/n^2 + 2k_{311}/n + 3k_{221}/n + k_{2111},$$
$$k_2 k_{11} k_1 = 2k_{41}/n^2 + 2(n-3)\,k_{32}/(nn^{(2)}) + 3k_{311}/n + 2(n-2)\,k_{221}/n^{(2)} + k_{2111},$$
$$k_{11} k_1^3 = 2k_{41}/n^3 + 6k_{32}/n^3 + 7k_{311}/n^2 + 12k_{221}/n^2 + 9k_{2111}/n + k_{11111},$$
$$k_{211} k_1 = k_{311}/n + 2k_{221}/n + k_{2111},$$
$$k_{21} k_{11} = 2k_{32}/n^{(2)} + 2k_{311}/n + 2(n-2)\,k_{221}/n^{(2)} + k_{2111},$$
$$k_2 k_{111} = 3k_{311}/n - 6k_{221}/n^{(2)} + k_{2111},$$
$$k_{111} k_1^2 = 3k_{311}/n^2 + 6k_{221}/n^2 + 7k_{2111}/n + k_{11111},$$
$$k_{11}^2 k_1 = 4k_{32}/(nn^{(2)}) + 4k_{311}/n^2 + 2(5n-4)\,k_{221}/(nn^{(2)}) + 8k_{2111}/n + k_{11111},$$
$$k_{1111} k_1 = 4k_{2111}/n + k_{11111},$$
$$k_{111} k_{11} = 6k_{221}/n^{(2)} + 6k_{2111}/n + k_{11111}.$$

6th order

$$
\begin{aligned}
k_5 k_1 &= k_6/n + k_{51},\\
k_4 k_2 &= k_6/n + (n+7)\, k_{42}/(n-1) + 6k_{33}/(n-1),\\
k_3^2 &= k_6/n + 9k_{42}/(n-1) + (n+8)\, k_{33}/(n-1) + 6nk_{222}/(n-1)^{(2)},\\
k_4 k_1^2 &= k_6/n^2 + 2k_{51}/n + k_{42}/n + k_{411},\\
k_3 k_2 k_1 &= k_6/n^2 + k_{51}/n + (n+5)\, k_{42}/n^{(2)} + (n+5)\, k_{33}/n^{(2)} + (n+5)\, k_{321}/(n-1),\\
k_2^3 &= k_6/n^2 + 3(n+3)\, k_{42}/n^{(2)} + 4n(n-2)\, k_{33}/(n^{(2)})^2 + (n+1)\,(n+3)\, k_{222}/(n-1)^2,\\
k_3 k_1^3 &= k_6/n^3 + 3k_{51}/n^2 + 3k_{42}/n^2 + k_{33}/n^2 + 3k_{411}/n + 3k_{321}/n + k_{3111},\\
k_2^2 k_1^2 &= k_6/n^3 + 2k_{51}/n^2 + (3n+1)\, k_{42}/(nn^{(2)}) + 2(n+1)\, k_{33}/(nn^{(2)}) + k_{411}/n + 4(n+1)\, k_{321}/n^{(2)}\\
&\quad + (n+1)\, k_{222}/n^{(2)} + (n+1)\, k_{2211}/(n-1),\\
k_2 k_1^4 &= k_6/n^4 + 4k_{51}/n^3 + 7k_{42}/n^3 + 4k_{33}/n^3 + 6k_{411}/n^2 + 16k_{321}/n^2 + 3k_{222}/n^2 + 4k_{3111}/n\\
&\quad + 6k_{2211}/n + k_{21111},\\
k_1^6 &= k_6/n^5 + 6k_{51}/n^4 + 15k_{42}/n^4 + 10k_{33}/n^4 + 15k_{411}/n^3 + 60k_{321}/n^3 + 15k_{222}/n^3\\
&\quad + 20k_{3111}/n^2 + 45k_{2211}/n^2 + 15k_{21111}/n + k_{111111}.
\end{aligned}
$$

$$
\begin{aligned}
k_{41} k_1 &= k_{51}/n + k_{42}/n + k_{411},\\
k_4 k_{11} &= 2k_{51}/n - 8k_{42}/n^{(2)} - 6k_{33}/n^{(2)} + k_{411},\\
k_{32} k_1 &= k_{42}/n + k_{33}/n + k_{321},\\
k_{31} k_2 &= k_{51}/n - 2k_{42}/n^{(2)} + k_{33}/n + (n+5)\, k_{321}/(n-1),\\
k_3 k_{21} &= k_{51}/n + (n-4)\, k_{42}/n^{(2)} - 3k_{33}/n^{(2)} + (n+5)\, k_{321}/(n-1) - 6nk_{222}/n^{(3)},\\
k_{22} k_2 &= 2k_{42}/n - 2k_{33}/n^{(2)} + (n+3)\, k_{222}/(n-1),\\
k_{31} k_1^2 &= k_{51}/n^2 + 2k_{42}/n^2 + k_{33}/n^2 + 2k_{411}/n + 3k_{321}/n + k_{3111},\\
k_3 k_{11} k_1 &= 2k_{51}/n^2 + 2(n-4)\, k_{42}/(nn^{(2)}) - 6k_{33}/(nn^{(2)}) + 3k_{411}/n + 2(n-4)\, k_{321}/n^{(2)} + k_{3111},\\
k_{22} k_1^2 &= 2k_{42}/n^2 + 2k_{33}/n^2 + 4k_{321}/n + k_{222}/n + k_{2211},\\
k_{21} k_2 k_1 &= k_{51}/n^2 + 2(n-2)\, k_{42}/(nn^{(2)}) + (n-3)\, k_{33}/(nn^{(2)}) + k_{411}/n + (3n-1)\, k_{321}/n^{(2)}\\
&\quad + (n+1)\, k_{222}/n^{(2)} + (n+1)\, k_{2211}/(n-1),\\
k_2^2 k_{11} &= 2k_{51}/n^2 - 8k_{42}/(nn^{(2)}) + 2(n^2-2n+3)\, k_{33}/(n^{(2)})^2 + k_{411}/n + 4(n+1)\, k_{321}/n^{(2)}\\
&\quad - 4n(n+1)\, k_{222}/(n^{(2)})^2 + (n+1)\, k_{2211}/(n-1),\\
k_{21} k_1^3 &= k_{51}/n^3 + 4k_{42}/n^3 + 3k_{33}/n^3 + 3k_{411}/n^2 + 13k_{321}/n^2 + 3k_{222}/n^2 + 3k_{3111}/n\\
&\quad + 6k_{2211}/n + k_{21111},\\
k_2 k_{11} k_1^2 &= 2k_{51}/n^3 + 4(n-2)\, k_{42}/(n^2 n^{(2)}) + 2(n-3)\, k_{33}/(n^2 n^{(2)}) + 5k_{411}/n^2 + 4(3n-5)\, k_{321}/(nn^{(2)})\\
&\quad + 2(n-2)\, k_{222}/(nn^{(2)}) + 4k_{3111}/n + (5n-7)\, k_{2211}/n^{(2)} + k_{21111},\\
k_{11} k_1^4 &= 2k_{51}/n^4 + 8k_{42}/n^4 + 6k_{33}/n^4 + 9k_{411}/n^3 + 44k_{321}/n^3 + 12k_{222}/n^3 + 16k_{3111}/n^2\\
&\quad + 39k_{2211}/n^2 + 14k_{21111}/n + k_{111111},\\
k_{311} k_1 &= k_{411}/n + 2k_{321}/n + k_{3111},\\
k_{31} k_{11} &= 2k_{42}/n^{(2)} + 2k_{411}/n + 2(n-4)\, k_{321}/n^{(2)} + k_{3111},\\
k_{221} k_1 &= 2k_{321}/n + k_{222}/n + k_{2211},\\
k_{22} k_{11} &= 2k_{33}/n^{(2)} + 4k_{321}/n - 4k_{222}/n^{(2)} + k_{2211},\\
k_3 k_{111} &= 3k_{411}/n - 18k_{321}/n^{(2)} + 12k_{222}/n^{(3)} + k_{3111},\\
k_{211} k_2 &= k_{411}/n + 2(n-3)\, k_{321}/n^{(2)} - 2k_{222}/n^{(2)} + (n+1)\, k_{2211}/(n-1),\\
k_{21}^2 &= k_{42}/n^{(2)} + k_{33}/n^{(2)} + k_{411}/n + 2(n-3)\, k_{321}/n^{(2)} + (n^2-n+4)\, k_{222}/n^{(3)}\\
&\quad + (n+1)\, k_{2211}/(n-1),\\
k_{211} k_1^2 &= k_{411}/n^2 + 6k_{321}/n^2 + 2k_{222}/n^2 + 2k_{3111}/n + 5k_{2211}/n + k_{21111},\\
k_{21} k_{11} k_1 &= 2k_{42}/(nn^{(2)}) + 2k_{33}/(nn^{(2)}) + 2k_{411}/n^2 + 2(5n-6)\, k_{321}/(nn^{(2)}) + 2(n-2)\, k_{222}/(nn^{(2)})\\
&\quad + 3k_{3111}/n + (5n-7)\, k_{2211}/n^{(2)} + k_{21111},
\end{aligned}
$$

$$
\begin{aligned}
k_2 k_{111} k_1 &= 3k_{411}/n^2 + 6(n-3)\, k_{321}/(nn^{(2)}) - 6k_{222}/(nn^{(2)}) + 4k_{3111}/n + 3(n-3)\, k_{2211}/n^{(2)} + k_{21111}, \\
k_2 k_{11}^2 &= 4k_{42}/(nn^{(2)}) - 4k_{33}/(n^{(2)})^2 + 4k_{411}/n^2 + 8(n-3)\, k_{321}/(nn^{(2)}) + 2(n^2-n+4)\, k_{222}/(n^{(2)})^2 \\
&\quad + 4k_{3111}/n + 4(n-2)\, k_{2211}/n^{(2)} + k_{21111}, \\
k_{111} k_1^3 &= 3k_{411}/n^3 + 18k_{321}/n^3 + 6k_{222}/n^3 + 10k_{3111}/n^2 + 27k_{2211}/n^2 + 12k_{21111}/n + k_{111111}, \\
k_{11}^2 k_1^2 &= 4k_{42}/(n^2n^{(2)}) + 4k_{33}/(n^2n^{(2)}) + 4k_{411}/n^3 + 8(4n-3)\, k_{321}/(n^2n^{(2)}) + 2(5n-4)\, k_{222}/(n^2n^{(2)}) \\
&\quad + 12k_{3111}/n^2 + 2(17n-16)\, k_{2211}/(nn^{(2)}) + 13k_{21111}/n + k_{111111}, \\
k_{2111} k_1 &= k_{3111}/n + 3k_{2211}/n + k_{21111}, \\
k_{211} k_{11} &= 4k_{321}/n^{(2)} + 2k_{222}/n^{(2)} + 2k_{3111}/n + 2(2n-3)\, k_{2211}/n^{(2)} + k_{21111}, \\
k_{21} k_{111} &= 6k_{321}/n^{(2)} - 6k_{222}/n^{(3)} + 3k_{3111}/n + 3(n-3)\, k_{2211}/n^{(2)} + k_{21111}, \\
k_2 k_{1111} &= 4k_{3111}/n - 12k_{2211}/n^{(2)} + k_{21111}, \\
k_{1111} k_1^2 &= 4k_{3111}/n^2 + 12k_{2211}/n^2 + 9k_{21111}/n + k_{111111}, \\
k_{111} k_{11} k_1 &= 12k_{321}/(nn^{(2)}) + 6k_{222}/(nn^{(2)}) + 6k_{3111}/n^2 + 6(4n-3)\, k_{2211}/(nn^{(2)}) \\
&\quad + 11k_{21111}/n + k_{111111}, \\
k_{11}^3 &= 4k_{33}/(n^{(2)})^2 + 24k_{321}/(nn^{(2)}) + 8(n-2)\, k_{222}/(n^{(2)})^2 + 8k_{3111}/n^2 \\
&\quad + 6(5n-4)\, k_{2211}/(nn^{(2)}) + 12k_{21111}/n + k_{111111}, \\
k_{11111} k_1 &= 5k_{21111}/n + k_{111111}, \\
k_{1111} k_{11} &= 12k_{2211}/n^{(2)} + 8k_{21111}/n + k_{111111}, \\
k_{111}^2 &= 6k_{222}/n^{(3)} + 18k_{2211}/n^{(2)} + 9k_{21111}/n + k_{111111}.
\end{aligned}
$$

7th order

$$
\begin{aligned}
k_6 k_1 &= k_7/n + k_{61}, \\
k_5 k_2 &= k_7/n + (n+9)\, k_{52}/(n-1) + 20k_{43}/(n-1), \\
k_4 k_3 &= k_7/n + 12k_{52}/(n-1) + (n+29)\, k_{43}/(n-1) + 36nk_{322}/(n-1)^{(2)}, \\
k_5 k_1^2 &= k_7/n^2 + 2k_{61}/n + k_{52}/n + k_{511}, \\
k_4 k_2 k_1 &= k_7/n^2 + k_{61}/n + (n+7)\, k_{52}/n^{(2)} + (n+19)\, k_{43}/n^{(2)} + (n+7)\, k_{421}/(n-1) + 6k_{331}/(n-1), \\
k_3^2 k_1 &= k_7/n^2 + k_{61}/n + 9k_{52}/n^{(2)} + (2n+25)\, k_{43}/n^{(2)} + 9k_{421}/(n-1) + (n+8)\, k_{331}/(n-1) \\
&\quad + 18k_{322}/(n-1)^{(2)} + 6nk_{2221}/(n-1)^{(2)}, \\
k_3 k_2^2 &= k_7/n^2 + 2(n+7)\, k_{52}/n^{(2)} + (n^2+22n-35)\, k_{43}/\{(n-1)\, n^{(2)}\} \\
&\quad + (n+5)\,(n+7)\, k_{322}/(n-1)^2, \\
k_4 k_1^3 &= k_7/n^3 + 3k_{61}/n^2 + 3k_{52}/n^2 + k_{43}/n^2 + 3k_{511}/n + 3k_{421}/n + k_{4111}, \\
k_3 k_2 k_1^2 &= k_7/n^3 + 2k_{61}/n^2 + 2(n+2)\, k_{52}/(nn^{(2)}) + 3(n+5)\, k_{43}/(nn^{(2)}) + k_{511}/n \\
&\quad + 2(n+5)\, k_{421}/n^{(2)} + 2(n+5)\, k_{331}/n^{(2)} + (n+5)\, k_{322}/n^{(2)} + (n+5)\, k_{3211}/(n-1), \\
k_2^3 k_1 &= k_7/n^3 + k_{61}/n^2 + 3(n+3)\, k_{52}/(nn^{(2)}) + (3n^2+14n-25)\, k_{43}/(n^{(2)})^2 + 3(n+3)\, k_{421}/n^{(2)} \\
&\quad + 4(n-2)\, k_{331}/\{(n-1)\, n^{(2)}\} + 3(n+1)\,(n+3)\, k_{322}/\{(n-1)\, n^{(2)}\} \\
&\quad + (n+1)\,(n+3)\, k_{2221}/(n-1)^2, \\
k_3 k_1^4 &= k_7/n^4 + 4k_{61}/n^3 + 6k_{52}/n^3 + 5k_{43}/n^3 + 6k_{511}/n^2 + 12k_{421}/n^2 + 4k_{331}/n^2 + 3k_{322}/n^2 \\
&\quad + 4k_{4111}/n + 6k_{3211}/n + k_{31111}, \\
k_2^2 k_1^3 &= k_7/n^4 + 3k_{61}/n^3 + (5n-1)\, k_{52}/(n^2n^{(2)}) + (7n+5)\, k_{43}/(n^2n^{(2)}) + 3k_{511}/n^2 \\
&\quad + 3(3n+1)\, k_{421}/(nn^{(2)}) + 6(n+1)\, k_{331}/(nn^{(2)}) + 7(n+1)\, k_{322}/(nn^{(2)}) + k_{4111}/n \\
&\quad + 6(n+1)\, k_{3211}/n^{(2)} + 3(n+1)\, k_{2221}/n^{(2)} + (n+1)\, k_{22111}/(n-1), \\
k_2 k_1^5 &= k_7/n^5 + 5k_{61}/n^4 + 11k_{52}/n^4 + 15k_{43}/n^4 + 10k_{511}/n^3 + 35k_{421}/n^3 + 20k_{331}/n^3 + 25k_{322}/n^3 \\
&\quad + 10k_{4111}/n^2 + 40k_{3211}/n^2 + 15k_{2221}/n^2 + 5k_{31111}/n + 10k_{22111}/n + k_{211111}, \\
k_1^7 &= k_7/n^6 + 7k_{61}/n^5 + 21k_{52}/n^5 + 35k_{43}/n^5 + 21k_{511}/n^4 + 105k_{421}/n^4 + 70k_{331}/n^4 + 105k_{322}/n^4 \\
&\quad + 35k_{4111}/n^3 + 210k_{3211}/n^3 + 105k_{2221}/n^3 + 35k_{31111}/n^2 + 105k_{22111}/n^2 \\
&\quad + 21k_{211111}/n + k_{1111111}.
\end{aligned}
$$

8th order

$$
\begin{aligned}
k_7 k_1 &= k_8/n + k_{71}, \\
k_6 k_2 &= k_8/n + (n+11)\,k_{62}/(n-1) + 30k_{53}/(n-1) + 20k_{44}/(n-1), \\
k_5 k_3 &= k_8/n + 15k_{62}/(n-1) + (n+44)\,k_{53}/(n-1) + 30k_{44}/(n-1) + 60nk_{422}/(n-1)^{(2)} \\
&\quad + 90nk_{332}/(n-1)^{(2)}, \\
k_4^2 &= k_8/n + 16k_{62}/(n-1) + 48k_{53}/(n-1) + (n+33)\,k_{44}/(n-1) + 72nk_{422}/(n-1)^{(2)} \\
&\quad + 144nk_{332}/(n-1)^{(2)} + 24n(n+1)\,k_{2222}/(n-1)^{(3)}, \\
k_6 k_1^2 &= k_8/n^2 + 2k_{71}/n + k_{62}/n + k_{611}, \\
k_5 k_2 k_1 &= k_8/n^2 + k_{71}/n + (n+9)\,k_{62}/n^{(2)} + (n+29)\,k_{53}/n^{(2)} + 20k_{44}/n^{(2)} + (n+9)\,k_{521}/(n-1) \\
&\quad + 20k_{431}/(n-1), \\
k_4 k_3 k_1 &= k_8/n^2 + k_{71}/n + 12k_{62}/n^{(2)} + (n+41)\,k_{53}/n^{(2)} + (n+29)\,k_{44}/n^{(2)} + 12k_{521}/(n-1) \\
&\quad + (n+29)\,k_{431}/(n-1) + 36k_{422}/(n-1)^{(2)} + 72k_{332}/(n-1)^{(2)} + 36nk_{3221}/(n-1)^{(2)}, \\
k_4 k_2^2 &= k_8/n^2 + 2(n+9)\,k_{62}/n^{(2)} + 8(5n-7)\,k_{53}/\{(n-1)\,n^{(2)}\} + (n^2+26n-39)\,k_{44}/\{(n-1)\,n^{(2)}\} \\
&\quad + (n+7)\,(n+9)\,k_{422}/(n-1)^2 + 12(n+9)\,k_{332}/(n-1)^2, \\
k_3^2 k_2 &= k_8/n^2 + (n+20)\,k_{62}/n^{(2)} + 2(n^2+22n-32)\,k_{53}/\{(n-1)\,n^{(2)}\} + 9(3n-5)\,k_{44}/\{(n-1)\,n^{(2)}\} \\
&\quad + 9(n^2+9n-20)\,k_{422}/\{(n-1)^2\,(n-2)\} \\
&\quad + (n^3+17n^2+104n-320)\,k_{332}/\{(n-1)^2\,(n-2)\} + 6n(n+5)\,k_{2222}/\{(n-1)^2\,(n-2)\}, \\
k_5 k_1^3 &= k_8/n^3 + 3k_{71}/n^2 + 3k_{62}/n^2 + k_{53}/n^2 + 3k_{611}/n + 3k_{521}/n + k_{5111}, \\
k_4 k_2 k_1^2 &= k_8/n^3 + 2k_{71}/n^2 + 2(n+3)\,k_{62}/(nn^{(2)}) + 2(n+13)\,k_{53}/(nn^{(2)}) + (n+19)\,k_{44}/(nn^{(2)}) \\
&\quad + k_{611}/n + 2(n+7)\,k_{521}/n^{(2)} + 2(n+19)\,k_{431}/n^{(2)} + (n+7)\,k_{422}/n^{(2)} + 6k_{332}/n^{(2)} \\
&\quad + (n+7)\,k_{4211}/(n-1) + 6k_{3311}/(n-1), \\
k_3^2 k_1^2 &= k_8/n^3 + 2k_{71}/n^2 + (n+8)\,k_{62}/(nn^{(2)}) + 2(n+17)\,k_{53}/(nn^{(2)}) + (2n+25)\,k_{44}/(nn^{(2)}) \\
&\quad + k_{611}/n + 18k_{521}/n^{(2)} + 2(2n+25)\,k_{431}/n^{(2)} + 9k_{422}/(n-1)^{(2)} + (n^2+6n+20)\,k_{332}/n^{(3)} \\
&\quad + 9k_{4211}/(n-1) + (n+8)\,k_{3311}/(n-1) + 36k_{3221}/(n-1)^{(2)} + 6k_{2222}/(n-1)^{(2)} \\
&\quad + 6nk_{22211}/(n-1)^{(2)}, \\
k_3 k_2^2 k_1 &= k_8/n^3 + k_{71}/n^2 + 2(n+7)\,k_{62}/(nn^{(2)}) + 4(n^2+14n-21)\,k_{53}/(n^{(2)})^2 \\
&\quad + (n^2+22n-35)\,k_{44}/(n^{(2)})^2 + 2(n+7)\,k_{521}/n^{(2)} + (n^2+22n-35)\,k_{431}/\{(n-1)\,n^{(2)}\} \\
&\quad + (n+5)\,(n+7)\,k_{422}/\{(n-1)\,n^{(2)}\} + 2(n+5)\,(n+7)\,k_{332}/\{(n-1)\,n^{(2)}\} \\
&\quad + (n+5)\,(n+7)\,k_{3221}/(n-1)^2, \\
k_2^4 &= k_8/n^3 + 4(n+5)\,k_{62}/(nn^{(2)}) + 32(n-2)\,k_{53}/(n^{(2)})^2 \\
&\quad + (3n^3+23n^2-63n+45)\,k_{44}/\{(n-1)\,(n^{(2)})^2\} + 6(n+3)\,(n+5)\,k_{422}/\{(n-1)\,n^{(2)}\} \\
&\quad + 16(n-2)\,(n+5)\,k_{332}/\{(n-1)^2\,n^{(2)}\} + (n+1)\,(n+3)\,(n+5)\,k_{2222}/(n-1)^3, \\
k_4 k_1^4 &= k_8/n^4 + 4k_{71}/n^3 + 6k_{62}/n^3 + 4k_{53}/n^3 + k_{44}/n^3 + 6k_{611}/n^2 + 12k_{521}/n^2 + 4k_{431}/n^2 \\
&\quad + 3k_{422}/n^2 + 4k_{5111}/n + 6k_{4211}/n + k_{41111}, \\
k_3 k_2 k_1^3 &= k_8/n^4 + 3k_{71}/n^3 + 2(2n+1)\,k_{62}/(n^2 n^{(2)}) + (5n+19)\,k_{53}/(n^2 n^{(2)}) + 3(n+5)\,k_{44}/(n^2 n^{(2)}) \\
&\quad + 3k_{611}/n^2 + 6(n+2)\,k_{521}/(nn^{(2)}) + 9(n+5)\,k_{431}/(nn^{(2)}) + 3(n+5)\,k_{422}/(nn^{(2)}) \\
&\quad + 4(n+5)\,k_{332}/(nn^{(2)}) + k_{5111}/n + 3(n+5)\,k_{4211}/n^{(2)} + 3(n+5)\,k_{3311}/n^{(2)} \\
&\quad + 3(n+5)\,k_{3221}/n^{(2)} + (n+5)\,k_{32111}/(n-1), \\
k_2^3 k_1^2 &= k_8/n^4 + 2k_{71}/n^3 + 4(n+2)\,k_{62}/(n^2 n^{(2)}) + 2(3n^2+10n-17)\,k_{53}/\{n(n^{(2)})^2\} \\
&\quad + (3n^2+14n-25)\,k_{44}/\{n(n^{(2)})^2\} + k_{611}/n^2 + 6(n+3)\,k_{521}/(nn^{(2)}) \\
&\quad + 2(3n^2+14n-25)\,k_{431}/(n^{(2)})^2 + 6(n+3)\,k_{422}/\{(n-1)\,n^{(2)}\} \\
&\quad + 2(3n^2+14n+5)\,k_{332}/(n^{(2)})^2 + 3(n+3)\,k_{4211}/n^{(2)} + 4(n-2)\,k_{3311}/\{(n-1)\,n^{(2)}\} \\
&\quad + 6(n+1)\,(n+3)\,k_{3221}/\{(n-1)\,n^{(2)}\} + (n+1)\,(n+3)\,k_{2222}/\{(n-1)\,n^{(2)}\} \\
&\quad + (n+1)\,(n+3)\,k_{22211}/(n-1)^2,
\end{aligned}
$$

$$k_3 k_1^5 = k_8/n^5 + 5k_{71}/n^4 + 10k_{62}/n^4 + 11k_{53}/n^4 + 5k_{44}/n^4 + 10k_{611}/n^3 + 30k_{521}/n^3 + 25k_{431}/n^3$$
$$+ 15k_{422}/n^3 + 10k_{332}/n^3 + 10k_{5111}/n^2 + 30k_{4211}/n^2 + 10k_{3311}/n^2 + 15k_{3221}/n^2 + 5k_{41111}/n$$
$$+ 10k_{32111}/n + k_{311111},$$

$$k_2^2 k_1^4 = k_8/n^5 + 4k_{71}/n^4 + 4(2n-1)\,k_{62}/(n^3 n^{(2)}) + 4(3n+1)\,k_{53}/(n^3 n^{(2)}) + (7n+5)\,k_{44}/(n^3 n^{(2)})$$
$$+ 6k_{611}/n^3 + 4(5n-1)\,k_{521}/(n^2 n^{(2)}) + 4(7n+5)\,k_{431}/(n^2 n^{(2)}) + 2(8n+5)\,k_{422}/(n^2 n^{(2)})$$
$$+ 20(n+1)\,k_{332}/(n^2 n^{(2)}) + 4k_{5111}/n^2 + 6(3n+1)\,k_{4211}/(nn^{(2)}) + 12(n+1)\,k_{3311}/(nn^{(2)})$$
$$+ 28(n+1)\,k_{3221}/(nn^{(2)}) + 3(n+1)\,k_{2222}/(nn^{(2)}) + k_{41111}/n + 8(n+1)\,k_{32111}/n^{(2)}$$
$$+ 6(n+1)\,k_{22211}/n^{(2)} + (n+1)\,k_{221111}/(n-1),$$

$$k_2 k_1^6 = k_8/n^6 + 6k_{71}/n^5 + 16k_{62}/n^5 + 26k_{53}/n^5 + 15k_{44}/n^5 + 15k_{611}/n^4 + 66k_{521}/n^4 + 90k_{431}/n^4$$
$$+ 60k_{422}/n^4 + 70k_{332}/n^4 + 20k_{5111}/n^3 + 105k_{4211}/n^3 + 60k_{3311}/n^3 + 150k_{3221}/n^3$$
$$+ 15k_{2222}/n^3 + 15k_{41111}/n^2 + 80k_{32111}/n^2 + 45k_{22211}/n^2 + 6k_{311111}/n$$
$$+ 15k_{221111}/n + k_{2111111},$$

$$k_1^8 = k_8/n^7 + 8k_{71}/n^6 + 28k_{62}/n^6 + 56k_{53}/n^6 + 35k_{44}/n^6 + 28k_{611}/n^5 + 168k_{521}/n^5$$
$$+ 280k_{431}/n^5 + 210k_{422}/n^5 + 280k_{332}/n^5 + 56k_{5111}/n^4 + 420k_{4211}/n^4 + 280k_{3311}/n^4$$
$$+ 840k_{3221}/n^4 + 105k_{2222}/n^4 + 70k_{41111}/n^3 + 560k_{32111}/n^3 + 420k_{22211}/n^3$$
$$+ 56k_{311111}/n^2 + 210k_{221111}/n^2 + 28k_{2111111}/n + k_{11111111}.$$

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